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MXene-Integrated Perovskite Tandem Solar Cells for Sustainable Development Goals (SDGs): A Bibliometric and Physics-Informed Artificial Intelligence (AI) Analysis Using Graph Neural Networks and Transformer Models

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ABSTRACT

This study presents a bibliometric and artificial intelligence (AI) analysis of MXene-integrated perovskite tandem solar cells to support renewable energy innovation and the Sustainable Development Goals (SDGs). A literature-based bibliometric perspective was used to identify research trends in perovskite tandem photovoltaics, MXene materials, and AI-assisted solar cell optimization. A physics-informed computational framework integrating Graph Neural Networks (GNNs) and Transformer models was then developed using 200 photovoltaic samples with 26 material, environmental, and performance variables. The GNN model captured nonlinear material–performance relationships, while the Transformer model predicted retention and degradation behavior under humidity and thermal stress. Feature importance analysis identified MXene loading, conductivity, defect density, and interface quality as dominant factors affecting efficiency and stability.

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1. INTRODUCTION

The global transition toward low-carbon energy systems has increased the demand for advanced photovoltaic technologies that are efficient, stable, scalable, and compatible with the Sustainable Development Goals (SDGs). Solar energy plays an important role in supporting SDG 7 on affordable and clean energy, SDG 9 on industry, innovation, and infrastructure, and SDG 13 on climate action. In this context, perovskite tandem solar cells have attracted major attention because they offer high power conversion efficiency, tunable bandgap, lightweight structure, and lower fabrication potential compared with conventional photovoltaic technologies. Recent developments in photovoltaic research have shown that tandem architectures can overcome the efficiency limitations of single-junction solar cells and provide pathways toward next-generation solar energy systems (Dale and Scarpulla, 2023; Green *et al.*, 2024; Kojima *et al.*, 2009; Aydin *et al.*, 2024).

Perovskite solar cells have demonstrated rapid progress since their early application as visible-light sensitizers in photovoltaic systems. Their unique optoelectronic properties, including strong light absorption, long carrier diffusion length, tunable bandgap, and compatibility with solution processing, make them promising candidates for high-efficiency solar cell technologies (Kojima *et al.*, 2009; Correa-Baena *et al.*, 2017). Perovskite–silicon tandem solar cells have also shown outstanding efficiency potential, with reported efficiencies exceeding 30% under laboratory conditions (Aydin *et al.*, 2024; Al-Ashouri *et al.*, 2020; Chin *et al.*, 2023). However, despite these achievements, perovskite tandem solar cells still face critical challenges related to thermal degradation, moisture sensitivity, ion migration, interface recombination, defect-induced carrier trapping, and reduced long-term operational stability (Snaith, 2018; Wang *et al.*, 2016; Niu *et al.*, 2015; Grätzel, 2014). These limitations restrict their practical commercialization and long-term contribution to sustainable energy deployment.

MXene materials, particularly Ti_3C_2Tx, have emerged as promising functional materials for improving perovskite solar cell performance. MXenes offer high electrical conductivity, large surface area, hydrophilic surface chemistry, superior carrier mobility, and defect passivation capability (Thakur *et al.*, 2025; Shahzad *et al.*, 2016). In perovskite-based photovoltaics, MXene-integrated layers can improve charge extraction, reduce recombination losses, enhance interfacial stability, and support better photovoltaic performance (Li *et al.*, 2021; Hui *et al.*, 2020). The comparison of tandem solar cell architecture, existing limitations, and MXene material advantages is presented in **Figure 1**. However, the nonlinear relationships among MXene concentration, conductivity, defect density, interface quality, environmental stress, and photovoltaic degradation remain difficult to understand using only conventional experimental approaches.

Artificial intelligence (AI) provides new opportunities for accelerating photovoltaic material analysis, performance prediction, and degradation modeling. Machine learning and deep learning approaches have been increasingly applied in solar energy systems for efficiency prediction, fault diagnosis, material screening, and system optimization (Ahmad *et al.*, 2021; Wang *et al.*, 2022; de la Asunción-Nadal *et al.*, 2025). Graph Neural Networks (GNNs) are especially relevant for photovoltaic material analysis because they can represent crystal structures, material similarity, and interface relationships as graph-based systems composed of nodes and edges (Xie and Grossman, 2018). Transformer models are also useful for analyzing sequential degradation behavior because their attention mechanisms can capture long-range dependencies and temporal changes in multivariable data (Lim *et al.*, 2021). These

AI models can support physics-informed photovoltaic prediction by connecting material properties, device structures, degradation conditions, and performance outputs (Raissi *et al.*, 2019; Karniadakis *et al.*, 2021).

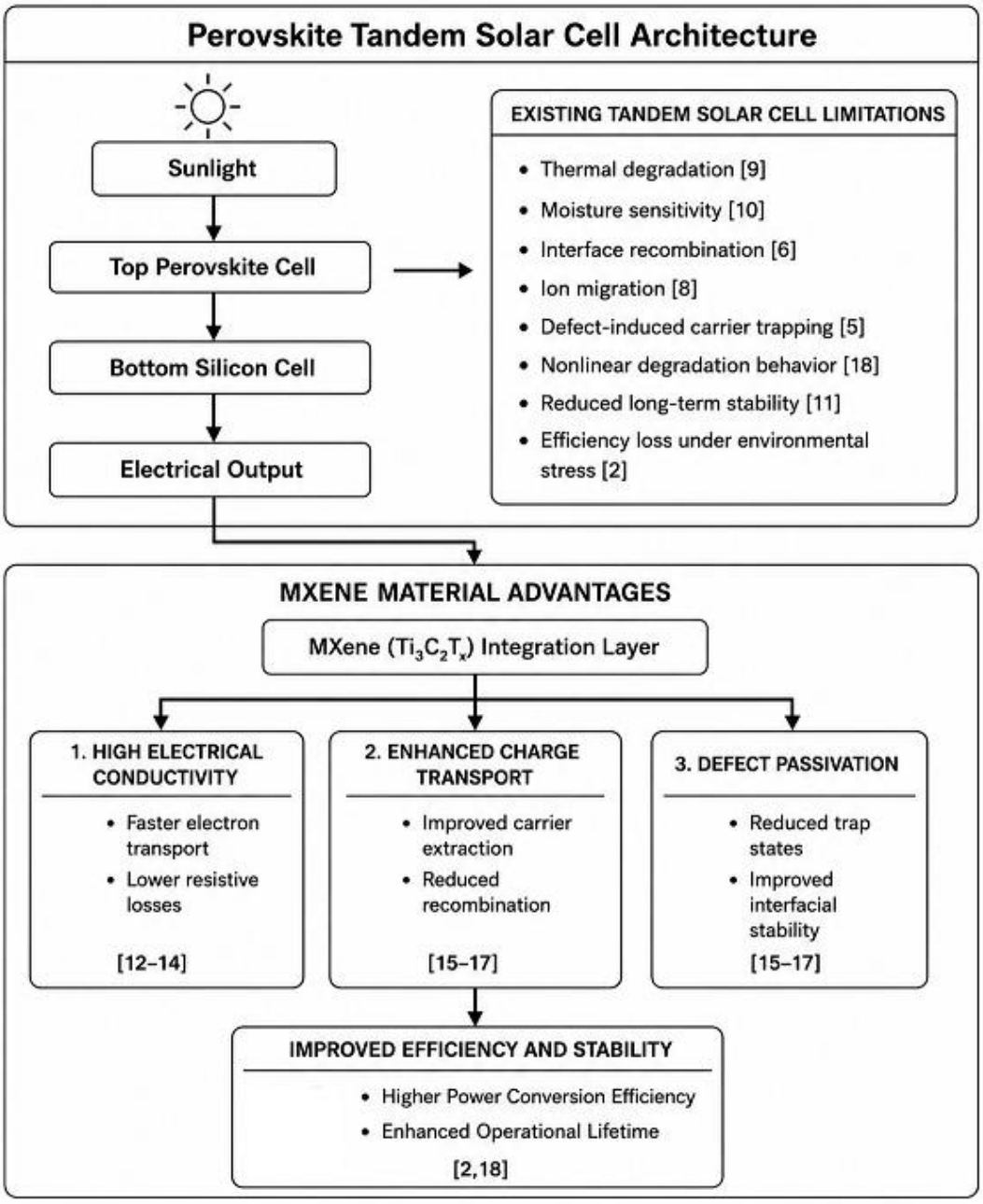

Figure 1. Comparison of perovskite tandem solar cell architecture with MXene material properties

Current studies on perovskite tandem solar cells, MXene-enhanced photovoltaic materials, and AI-assisted solar cell optimization have developed rapidly, but their integration remains limited. Previous works have discussed tandem photovoltaic efficiency, MXene applications, machine learning-assisted perovskite photovoltaics, crystal GNNs, and Transformer-based prediction models separately (Hou *et al.*, 2020; Shah *et al.*, 2021; Heo *et al.*, 2022; Torlao and

Fajardo, 2025). However, fewer studies combine MXene-enhanced tandem solar cell design, GNN-based structural learning, Transformer-based degradation prediction, and explainable AI within a unified framework for SDG-oriented photovoltaic technology development.

Based on this gap, this study develops a bibliometric and physics-informed AI framework for analyzing MXene-integrated perovskite tandem solar cells using GNNs and Transformer models. The study used a photovoltaic dataset containing 200 samples and 26 variables related to material composition, device architecture, environmental aging, electrical performance, defect behavior, charge transport, and stability retention. The novelty of this study lies in integrating bibliometric insight, MXene-enhanced tandem photovoltaic analysis, GNN-based graph representation, Transformer-based degradation prediction, and feature importance interpretation within a single AI-driven framework. This integrated approach is expected to support intelligent optimization, long-term stability assessment, and SDG-oriented development of next-generation solar cell technologies.

2. LITERATURE REVIEW

Perovskite tandem solar cells have become one of the most promising photovoltaic technologies because they can use complementary absorber layers to capture a broader solar spectrum. In tandem architectures, the top perovskite cell absorbs high-energy photons, while the bottom silicon or narrow-bandgap cell captures lower-energy photons. This design improves spectral utilization and enables higher efficiency than conventional single-junction solar cells (Dale and Scarpulla, 2023; Green *et al.*, 2024; Aydin *et al.*, 2024). Early perovskite photovoltaic research demonstrated the potential of organometal halide perovskites as visible-light sensitizers, and later studies showed rapid improvements in device efficiency, material engineering, and tandem integration (Kojima *et al.*, 2009; Correa-Baena *et al.*, 2017). The perovskite–silicon tandem architecture, bandgap engineering strategy, and efficiency development trend are illustrated in **Figure 2**.

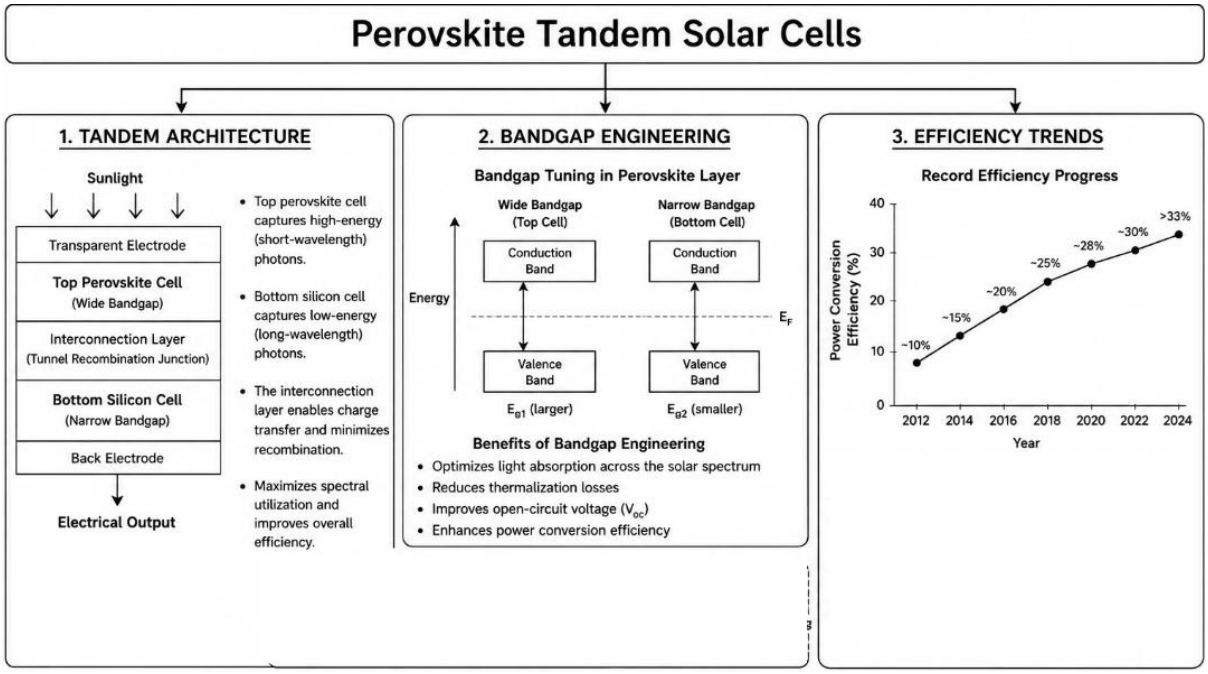

Figure 2. Perovskite–silicon tandem architecture, bandgap engineering, and efficiency trends

Despite their high efficiency potential, perovskite tandem solar cells continue to face major stability challenges. Thermal stress, humidity, oxygen exposure, ion migration, and interfacial recombination can accelerate degradation and reduce long-term device performance (Snaith, 2018; Wang *et al.*, 2016; Niu *et al.*, 2015; Grätzel, 2014). These degradation mechanisms are complex because they involve interactions among material composition, fabrication conditions, defect density, charge transport, and environmental exposure. Therefore, improving perovskite tandem solar cells requires not only better material design but also computational tools capable of predicting nonlinear degradation pathways and identifying dominant factors affecting device efficiency and stability.

MXenes have gained increasing attention as functional materials for photovoltaic and energy applications. Ti_3C_2Tx MXene is particularly attractive because of its high electrical conductivity, tunable surface termination, hydrophilic nature, and ability to improve interfacial charge transport (Thakur *et al.*, 2025). MXene-based materials have been widely explored in energy storage, catalysis, electromagnetic shielding, and photovoltaic applications (Shahzad *et al.*, 2016; Li *et al.*, 2021; Hui *et al.*, 2020). In perovskite solar cells, MXene can act as an additive, charge transport enhancer, passivation agent, or interfacial modification layer. These functions can reduce trap states, improve carrier extraction, decrease recombination, and enhance operational stability (Shah *et al.*, 2021; Heo *et al.*, 2022). The role of MXene-integrated materials in conductivity enhancement and interfacial engineering is shown in **Figure 3**.

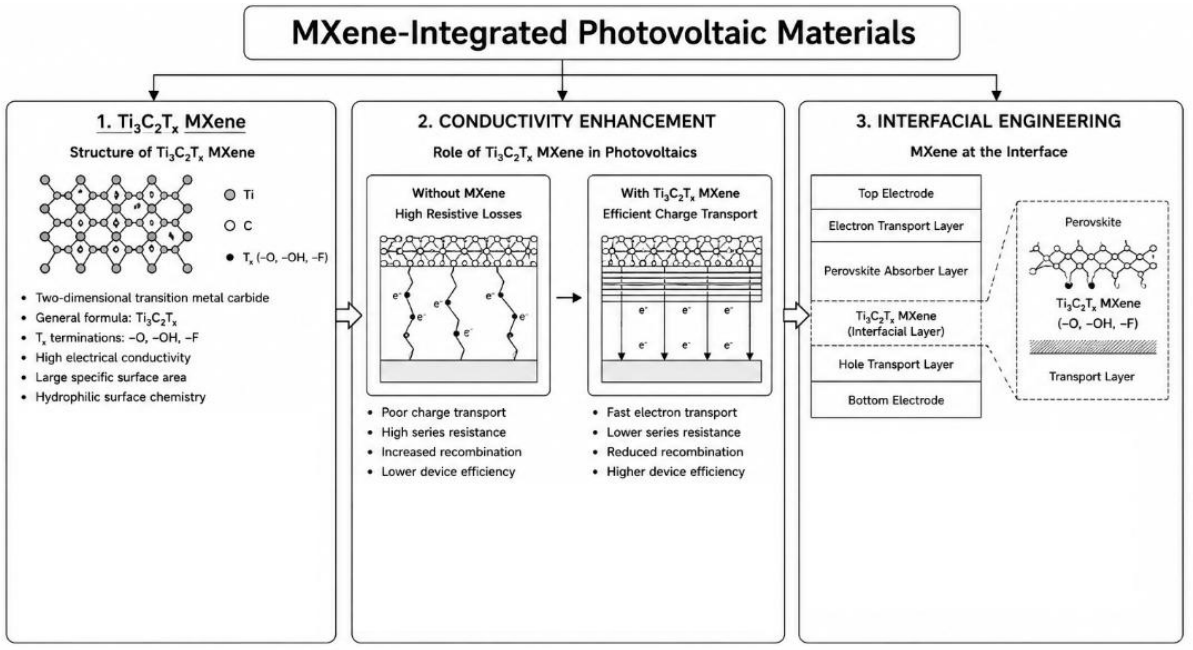

Figure 3. MXene-integrated material

Several studies have reported the benefits of MXene integration in perovskite solar cells. Some researchers (Shah *et al.*, 2021) reviewed the role of MXenes in perovskite solar cells and highlighted their potential for charge transport and interface engineering. Oxidized Ti_3C_2Tx MXene could support defect passivation and improve stability in $CsPbI_3$ perovskite solar cells (Heo *et al.*, 2022). Glycine-functionalized Ti_3C_2Tx MXene improved material properties and supported defect passivation in tin halide perovskite solar cells (Dizayee *et al.*, 2025). In tandem devices, high-efficiency benchmarks have been reported through enhanced hole extraction, interface passivation, and improved perovskite–silicon integration (Al-

Ashouri *et al.*, 2020; Chin *et al.*, 2023). MXene-based strategies have strong potential for improving both efficiency and stability, but systematic prediction of material–performance relationships remains necessary.

AI has become an important tool for accelerating research in photovoltaic materials and renewable energy systems. AI-assisted methods can reduce experimental costs, identify hidden patterns, optimize device parameters, and predict long-term performance under complex operating conditions (Ahmad *et al.*, 2021; Mousavi *et al.*, 2025). Machine learning-assisted strategies have been used for next-generation perovskite photovoltaics, including material discovery, device optimization, stability analysis, and performance prediction (de la Asunción-Nadal *et al.*, 2025). Deep learning methods have also been applied to intelligent fault diagnosis and photovoltaic performance prediction, showing their usefulness in renewable energy monitoring and optimization (Wang *et al.*, 2022).

GNNs are suitable for material and photovoltaic analysis because they can model relational structures. In graph-based learning, materials, devices, or samples can be represented as nodes, while their similarities or interactions can be represented as edges. This allows GNNs to capture nonlinear relationships between structural features and target properties. Crystal Graph Convolutional Neural Networks have shown strong capability for predicting material properties from crystal structures and atomic arrangements (Xie and Grossman, 2018). SchNet and Atomistic Line GNNs further demonstrate that graph-based deep learning can model molecules, crystals, and materials through node-edge interactions and message-passing operations (Schütt *et al.*, 2018; Choudhary and DeCost, 2021). In the context of MXene-integrated perovskite tandem solar cells, GNNs can be used to learn relationships among MXene loading, conductivity, defect density, interface quality, device structure, and power conversion efficiency.

Transformer models provide another important approach for photovoltaic degradation prediction. Unlike conventional sequence models, Transformer architectures use self-attention mechanisms to identify important variables and long-range dependencies across sequential data. Temporal Fusion Transformers have also shown strong performance in interpretable multi-horizon time series forecasting, making them relevant for degradation prediction and retention modeling (Lim *et al.*, 2021). In photovoltaic systems, degradation behavior often depends on environmental stress, aging duration, humidity, temperature, illumination intensity, and material stability. Therefore, Transformer models can help predict retention behavior and long-term performance changes under varying operating conditions.

Physics-informed machine learning offers an additional advantage by combining data-driven prediction with scientific constraints. Physics-informed neural networks and physics-informed machine learning frameworks have been used to solve forward and inverse problems in nonlinear systems and to improve interpretability in scientific modeling (Raissi *et al.*, 2019; Karniadakis *et al.*, 2021). In photovoltaic research, physics-informed AI can help ensure that predictions remain consistent with known relationships among material properties, electrical outputs, degradation mechanisms, and device performance. This is important because purely data-driven models may produce accurate predictions but weak physical interpretation if they are not guided by domain knowledge.

Perovskite tandem solar cells, MXene materials, GNN models, Transformer models, and physics-informed AI have each been studied in different research streams. However, their integration for MXene-enhanced perovskite tandem solar cell optimization remains limited.

Existing studies tend to focus separately on tandem device efficiency, MXene interface engineering, machine learning-assisted perovskite screening, graph-based material prediction, or sequential forecasting. Therefore, an integrated framework is needed to connect material composition, device architecture, environmental stress, photovoltaic performance, degradation behavior, and explainable AI analysis. Such a framework can contribute not only to next-generation photovoltaic research but also to SDG-oriented renewable energy development by supporting cleaner, more efficient, and more durable solar cell technologies.

3. METHODOLOGY

This study used a bibliometric and physics-informed AI approach to analyze MXene-integrated perovskite tandem solar cells. The method combined bibliometric insight, literature-based dataset construction, synthetic data augmentation, GNN modeling, Transformer-based degradation prediction, and feature importance analysis. This approach was designed to support intelligent photovoltaic optimization and SDG-oriented renewable energy development, particularly SDG 7, SDG 9, and SDG 13.

The bibliometric stage was used to identify research trends and gaps related to perovskite tandem solar cells, MXene materials, AI, GNN models, Transformer models, and photovoltaic degradation prediction. Previous studies on perovskite tandem photovoltaics, MXene-enhanced solar cells, machine learning-assisted perovskite systems, graph-based material prediction, and Transformer-based forecasting were used as the conceptual basis for dataset and model development (Aydin *et al.*, 2024; Shah *et al.*, 2021; Heo *et al.*, 2022; de la Asunción-Nadal *et al.*, 2025; Xie and Grossman, 2018; Lim *et al.*, 2021).

A physics-guided photovoltaic dataset was developed using 200 samples and 26 variables. The variables covered device identification, tandem architecture, MXene type, surface termination, MXene functional role, interface passivation, perovskite bandgap, MXene loading, layer thickness, annealing temperature, humidity, aging temperature, illumination intensity, testing duration, open-circuit voltage, short-circuit current density, fill factor, power conversion efficiency, trap density, carrier mobility, conductivity, recombination rate, thermal degradation index, retention percentage, and stability class. The variable grouping is shown in **Figure 4**.

Synthetic data augmentation and parameter randomization were applied to increase dataset variability while maintaining physically meaningful relationships among MXene concentration, conductivity, defect density, interface quality, environmental stress, and photovoltaic performance. Data preprocessing included normalization, feature scaling, graph construction, and sequence preparation. The GNN and Transformer training workflow is shown in **Figure 5**, while the model architecture for retention prediction is shown in **Figure 6**.

The GNN model was used to learn structural and relational patterns among photovoltaic material variables. Photovoltaic samples and material features were represented as graph structures consisting of nodes and edges. The GNN applied message-passing operations to capture nonlinear relationships among MXene loading, conductivity, defect density, interface quality, and power conversion efficiency (Xie and Grossman, 2018; Schütt *et al.*, 2018; Choudhary and DeCost, 2021).

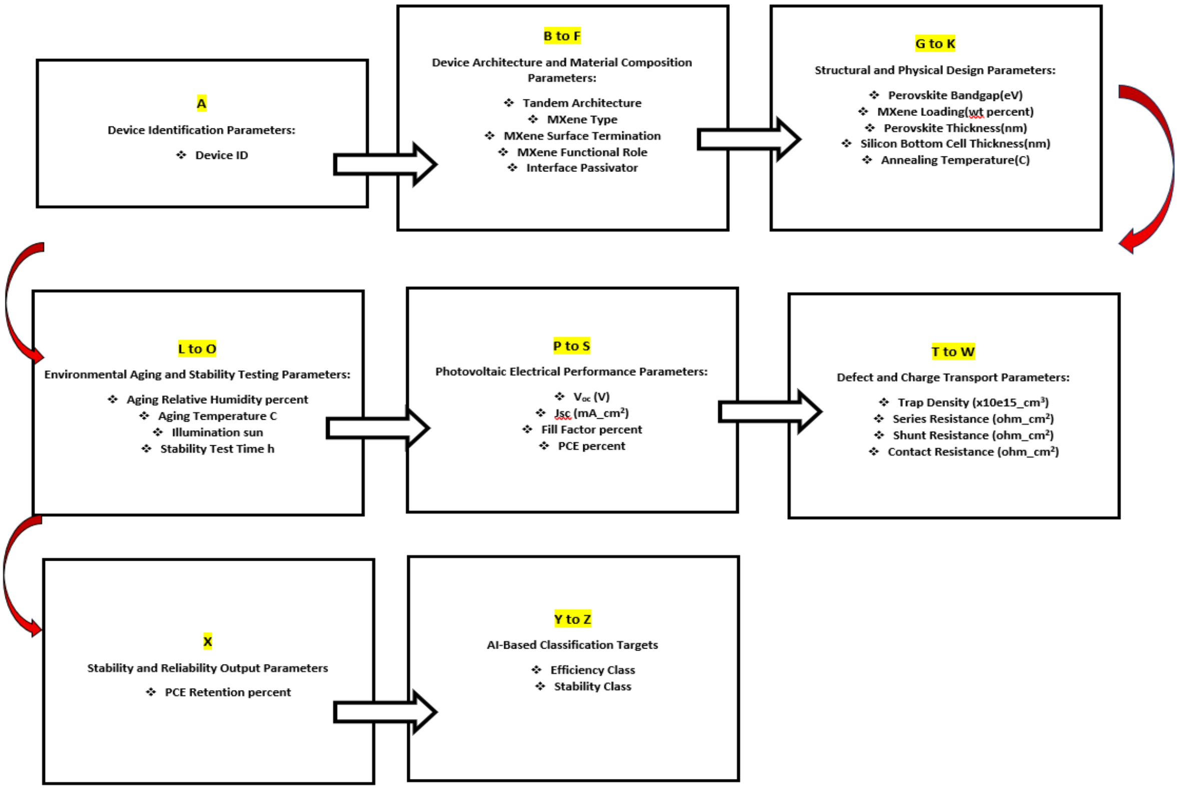

Figure 4. Description of 26 variables in dataset grouped into eight categories

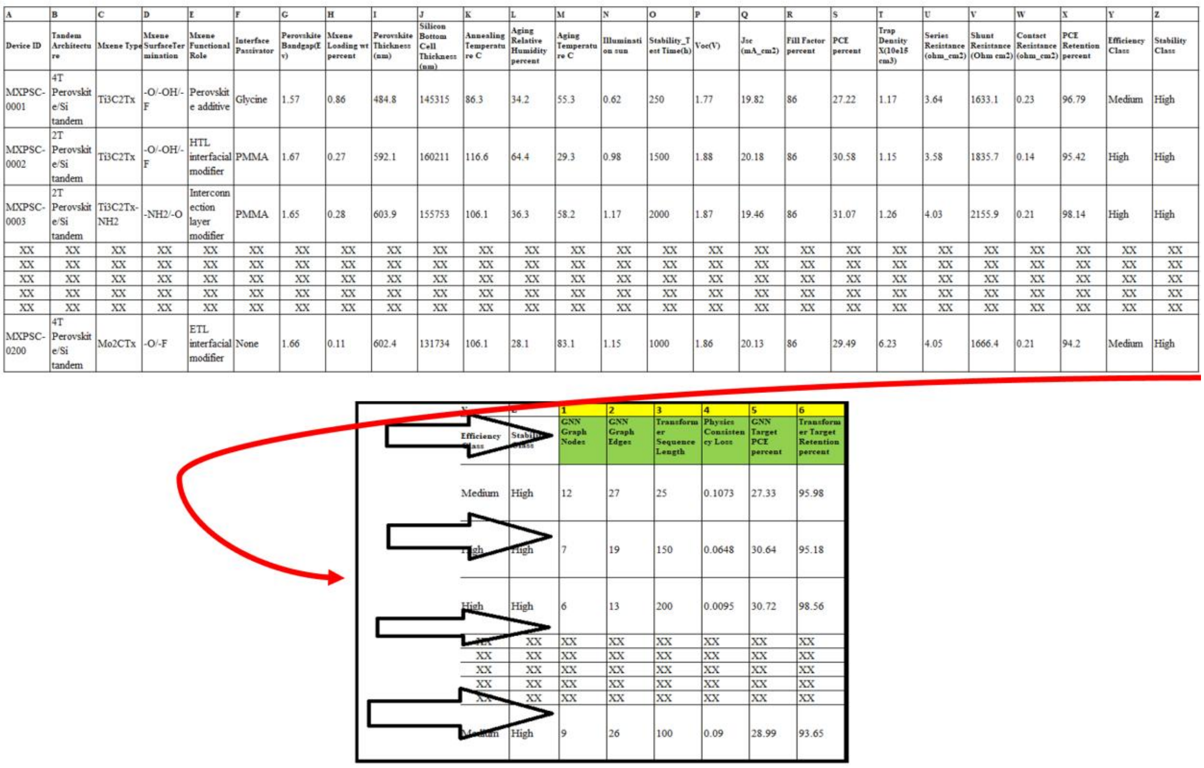

Figure 5. Training process workflow of GNN and Transformer models for 200 device-ID dataset samples

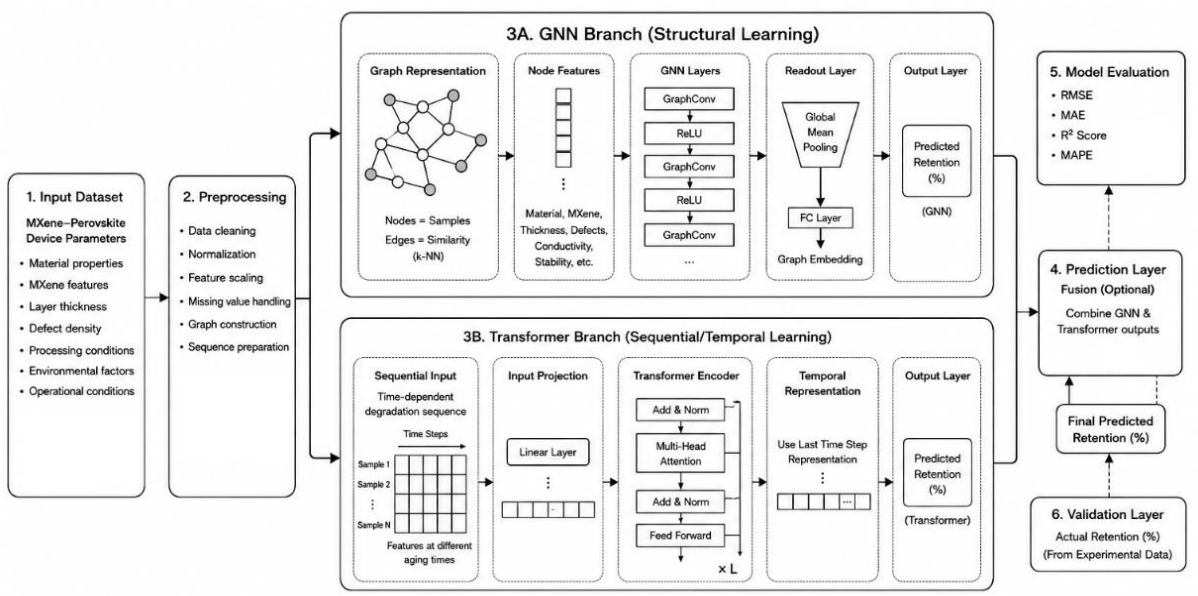

Figure 6. Model architecture for GNN and Transformer model for retention prediction

The Transformer model was used to predict stability retention and degradation behavior under humidity, temperature, illumination, and aging conditions. Its self-attention mechanism was applied to identify important temporal and environmental factors affecting photovoltaic degradation (Lim *et al.*, 2021). Physics-informed constraints were included to ensure that model predictions remained consistent with photovoltaic principles, including charge transport, defect density, recombination rate, power conversion efficiency, and degradation mechanisms (Raissi *et al.*, 2019; Karniadakis *et al.*, 2021).

Model performance was evaluated using root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2). Feature importance analysis was conducted to identify the dominant parameters affecting power conversion efficiency and stability retention, including MXene loading, conductivity, defect density, interface quality, and environmental stress.

4. RESULTS AND DISCUSSION

The bibliometric analysis was conducted using the Scopus database with the search query TITLE-ABS-KEY (perovskite AND tandem AND solar AND cells). The search covered publications from 2004 to 2025 and identified 3,810 documents. The annual publication trend is presented in **Figure 7**. The bibliometric result shows a strong and continuous increase in research related to perovskite tandem solar cells. In the early period from 2004 to 2013, the number of publications was very limited. A clear increase started after 2014 and became more rapid after 2018. The number of documents increased from 129 in 2017 to 201 in 2018, 305 in 2020, 340 in 2021, 425 in 2022, 530 in 2023, 651 in 2024, and 861 in 2025. Perovskite tandem solar cells have become an increasingly important topic in next-generation photovoltaic research. The rapid publication growth also supports the relevance of this study because high-efficiency and stable tandem solar cells are directly related to renewable energy development, SDG 7 on affordable and clean energy, SDG 9 on industry, innovation, and infrastructure, and SDG 13 on climate action.

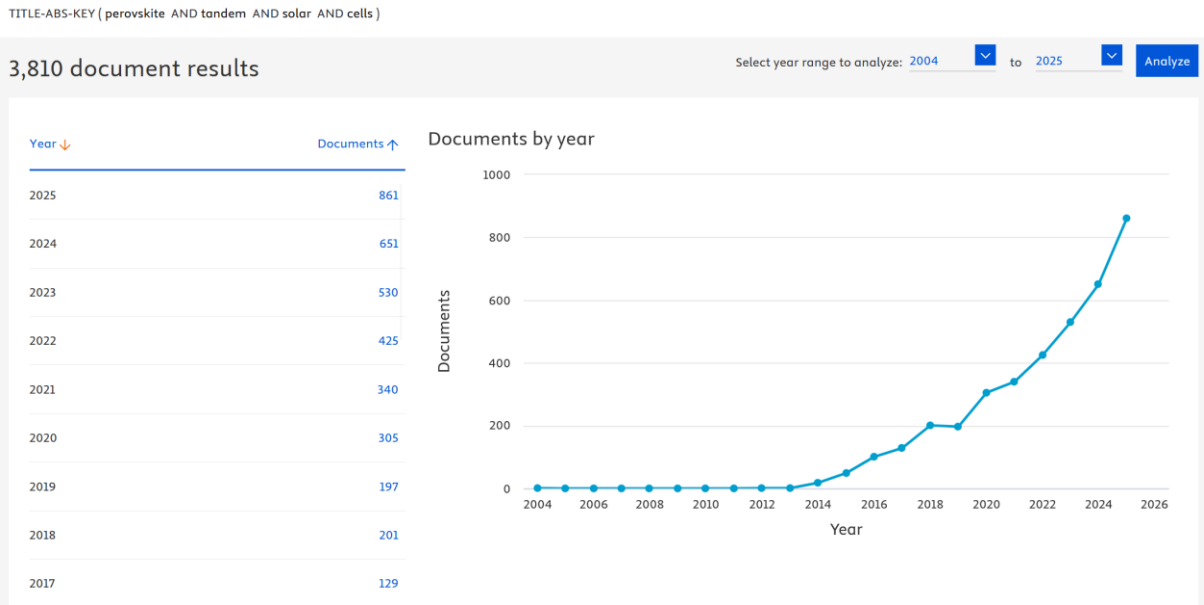

Figure 7. Bibliometric trend of publications on perovskite tandem solar cells based on Scopus data from 2004 to 2025.

Although the bibliometric trend shows rapid growth, the integration of perovskite tandem solar cells with MXene materials, GNNs, Transformer models, and physics-informed degradation prediction remains limited. Therefore, this study contributes to the field by combining bibliometric insight, MXene-enhanced photovoltaic materials, and AI-based prediction to analyze photovoltaic efficiency and stability.

The developed physics-informed AI framework demonstrated strong capability in predicting photovoltaic performance and retention behavior of MXene-integrated perovskite tandem solar cells. The dataset consisted of 200 samples and 26 variables representing material composition, device structure, fabrication conditions, environmental aging, electrical performance, defect behavior, charge transport, and stability retention. The integration of these variables enabled the models to capture complex relationships among MXene loading, conductivity, defect density, interface quality, environmental stress, and power conversion efficiency.

The GNN model was used to learn structural and relational patterns within the MXene–perovskite tandem solar cell dataset. The photovoltaic data were represented as graph structures consisting of nodes and edges, where nodes described material or device features and edges represented similarity relationships among samples. The KNN-based graph structure generated using NetworkX is shown in **Figure 8**. The dataset forms an interconnected network, indicating that material and device parameters are related through similarity patterns. Such graph representation is useful for identifying nonlinear relationships among photovoltaic variables.

A graph representation for the first 100 nodes is shown in **Figure 9**. This figure illustrates material similarity patterns among selected MXene-integrated perovskite tandem solar cell samples. Several device configurations share similar material, structural, or performance characteristics. This result supports the use of GNNs because graph-based learning can capture hidden relationships among MXene concentration, conductivity, defect density, interface quality, and photovoltaic performance.

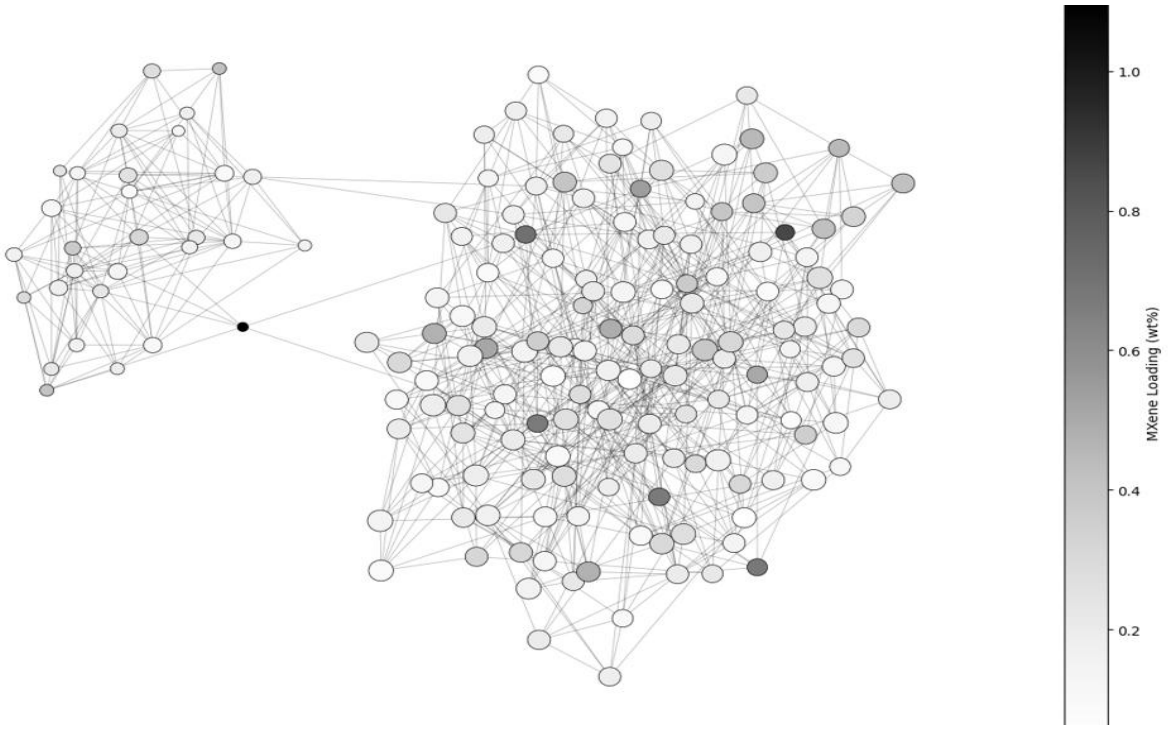

Figure 8. GNN graph structure of nodes and edges using KNN similarity and NetworkX.

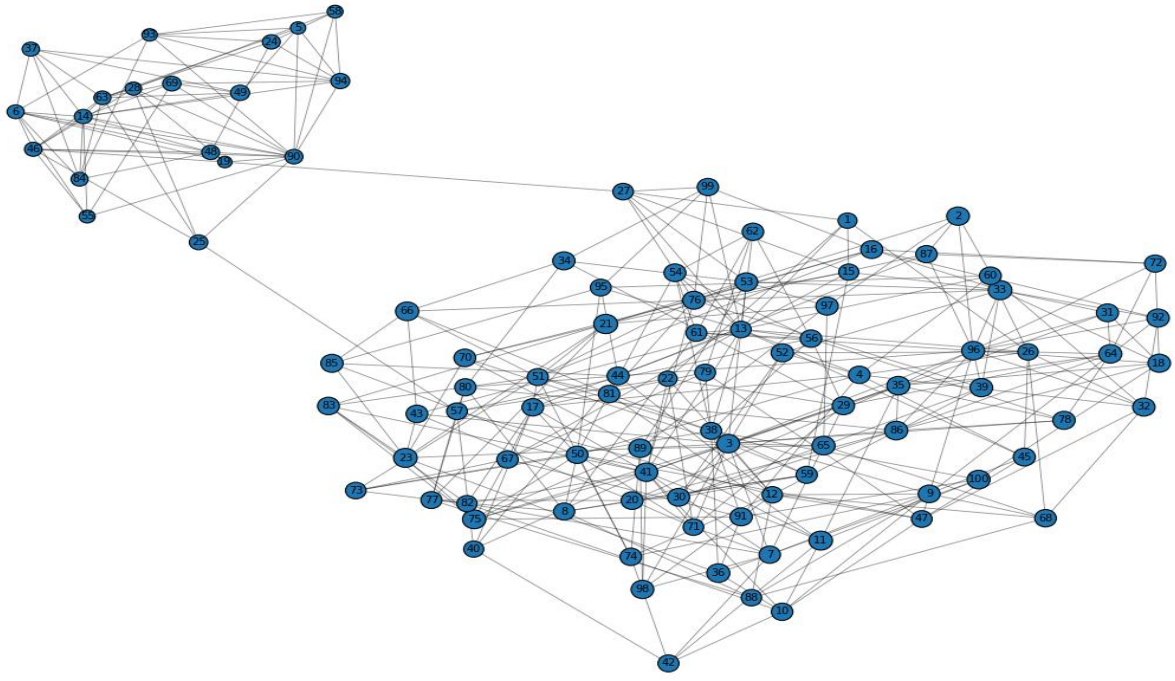

Figure 9. GNN graph structure showing material similarity for the first 100 nodes using NetworkX.

The complete graph structure of the MXene-integrated perovskite tandem dataset is shown in **Figure 10**. The network topology indicates that the dataset contains clustered and interconnected photovoltaic configurations. Certain combinations of MXene loading, interfacial properties, and degradation-related parameters may lead to similar photovoltaic responses. The graph-based approach can organize complex multivariable photovoltaic data into interpretable relational structures.

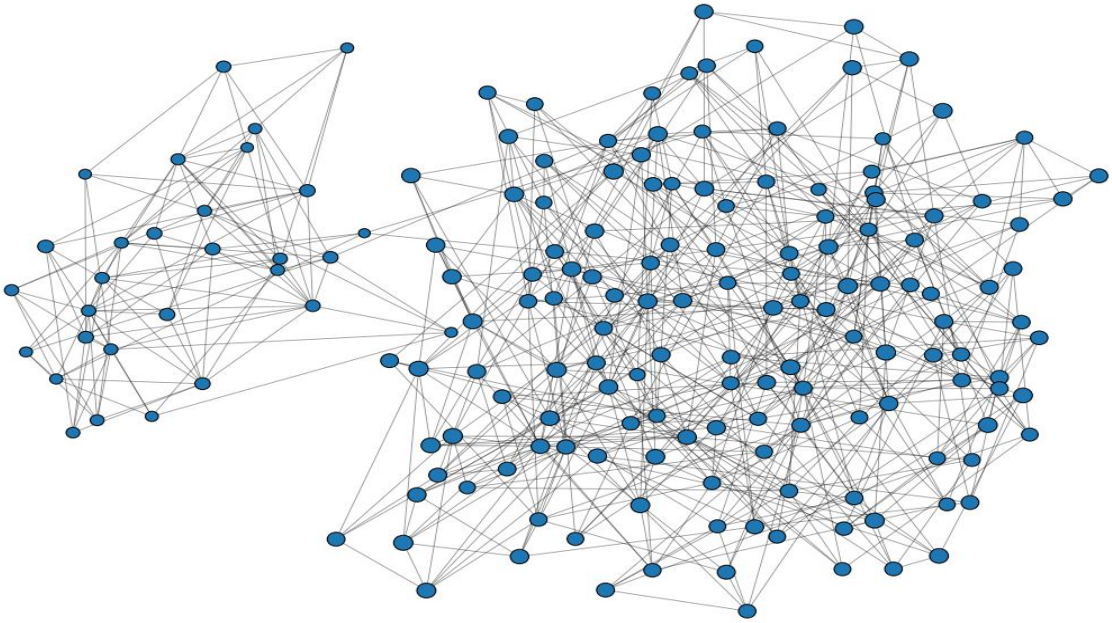

Figure 10. GNN graph structure of nodes for the MXene-integrated perovskite tandem dataset using NetworkX.

The comparative model performance is presented in **Figure 11**. The GNN model achieved lower RMSE and MAE values than the Transformer model, while also producing a higher coefficient of determination. Graph-based structural learning was more effective for predicting power conversion efficiency because it could capture nonlinear relationships among material composition, MXene loading, conductivity, defect density, and interfacial properties. In contrast, the Transformer model showed stronger relevance for sequential prediction of retention behavior because it was designed to capture temporal degradation patterns.

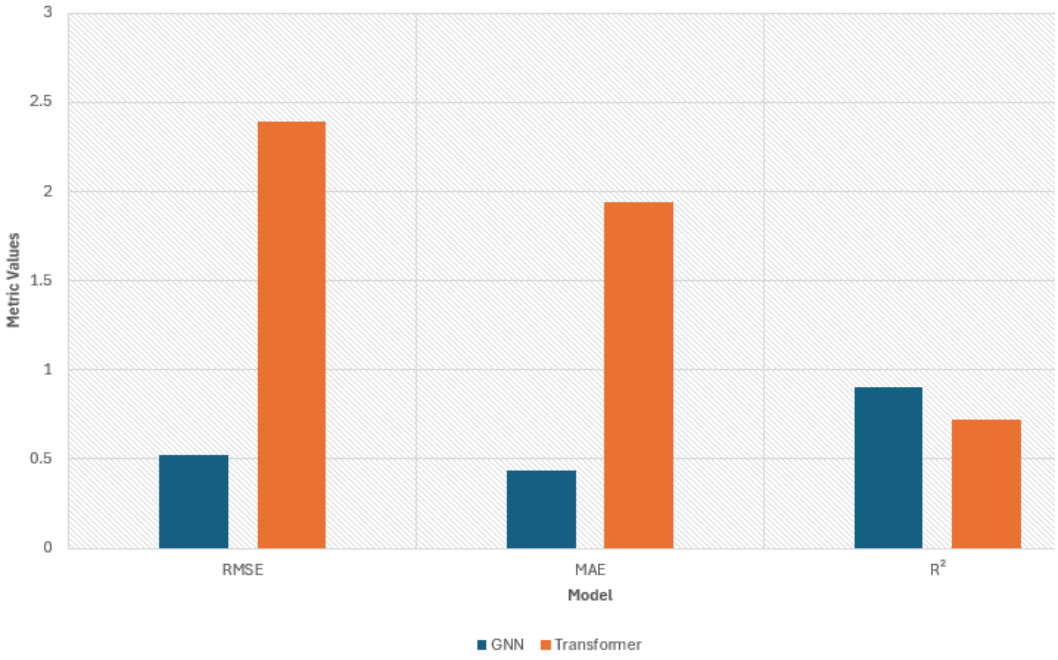

Figure 11. Model performance comparison between GNN and Transformer models.

The GNN prediction accuracy for photovoltaic efficiency is shown in **Figure 12**. The predicted power conversion efficiency values were close to the actual values, indicating that the GNN model successfully learned nonlinear relationships between input variables and photovoltaic performance. The model achieved low prediction errors and a high coefficient of determination, with R^2 approximately 0.90. GNN-based learning is suitable for modeling material–performance relationships in MXene-integrated perovskite tandem solar cells.

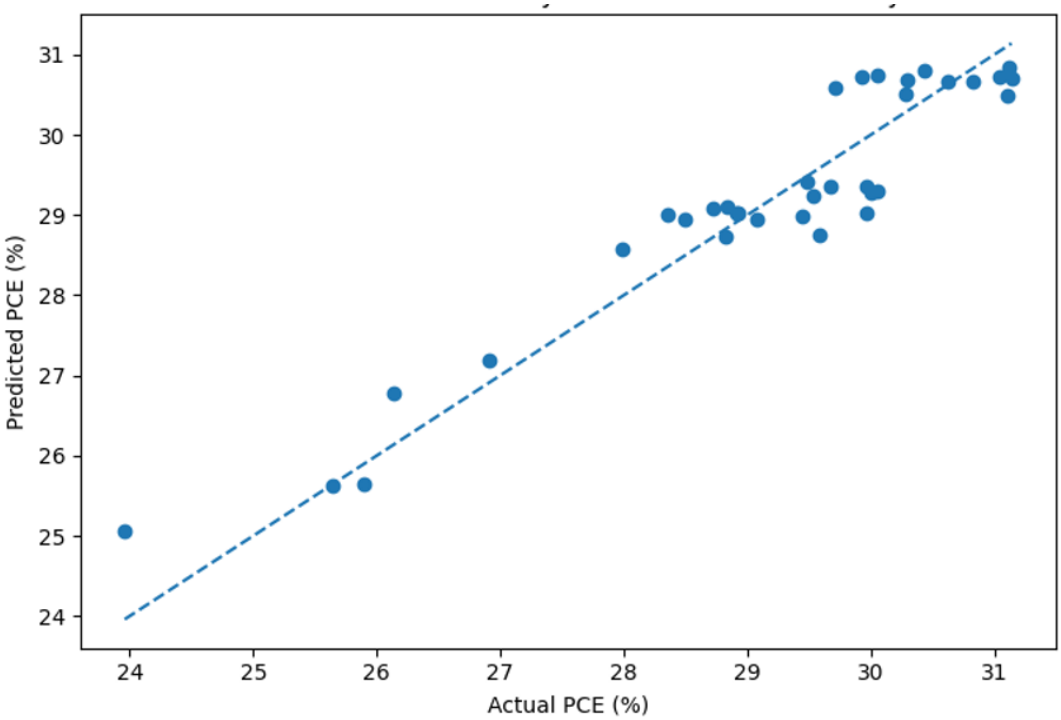

Figure 12. GNN prediction accuracy for photovoltaic efficiency.

The Transformer prediction accuracy for stability retention is shown in **Figure 13**. The predicted retention values closely followed the actual retention values, especially in the high-stability region. Minor deviations were observed under more severe degradation conditions caused by humidity and thermal stress. The Transformer model can capture sequential degradation patterns and temporal photovoltaic behavior through its self-attention mechanism. Therefore, the Transformer model is suitable for predicting long-term stability and retention behavior in next-generation tandem solar cells.

Feature importance analysis was conducted to identify the dominant parameters affecting photovoltaic efficiency and stability retention. The results are shown in **Figure 14**. MXene loading, conductivity, defect density, interface quality, stability class, humidity, aging temperature, and testing duration appeared as important factors influencing model prediction. These findings are scientifically reasonable because MXene concentration and conductivity affect charge transport, while defect density and interface quality influence recombination losses and carrier extraction. Environmental stress factors, such as humidity and temperature, strongly affect stability retention and degradation behavior.

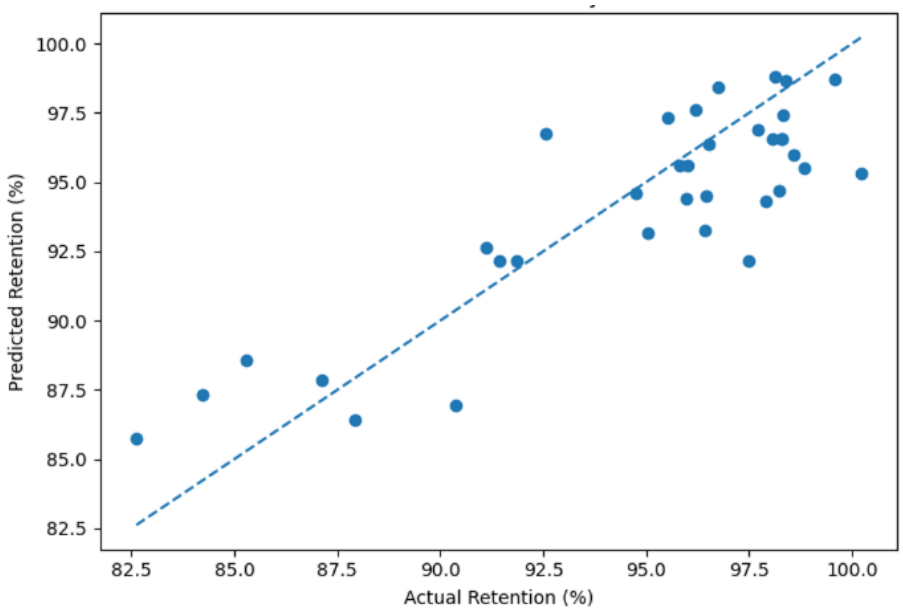

Figure 13. Transformer prediction accuracy for stability retention.

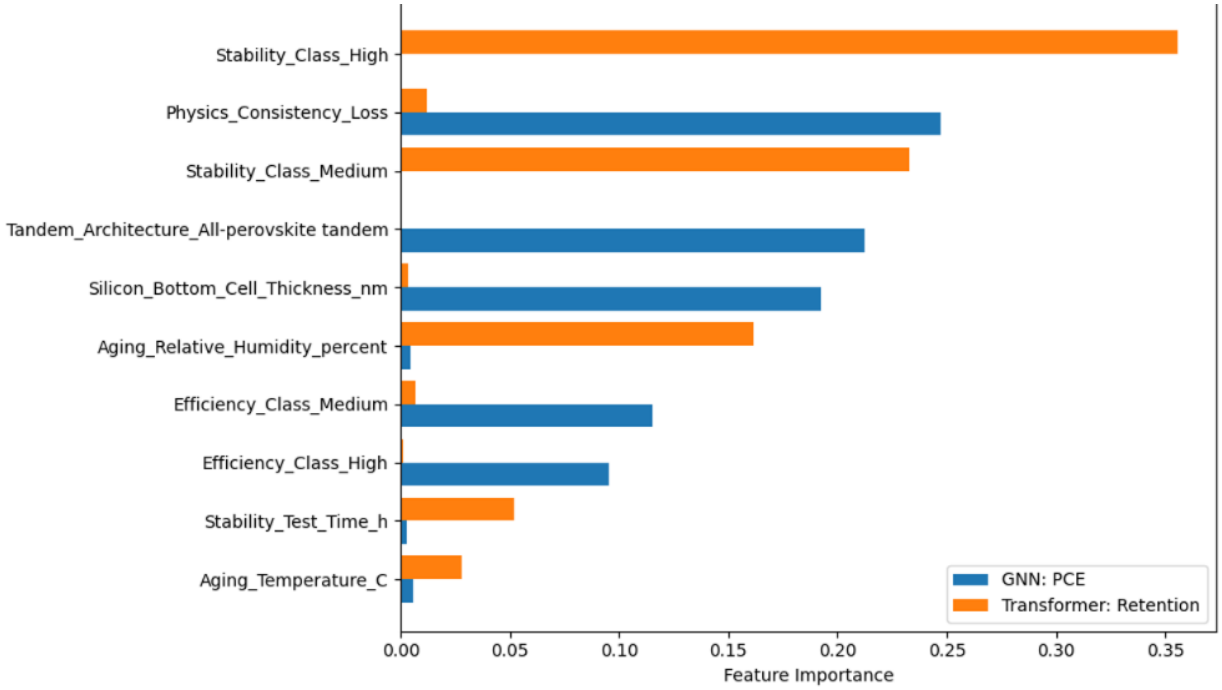

Figure 14. Feature importance analysis for GNN and Transformer models.

The proposed hybrid physics-informed AI framework can support intelligent optimization of MXene-integrated perovskite tandem solar cells. The bibliometric analysis confirms the rapid growth of perovskite tandem solar cell research, while the AI-based results demonstrate that GNN and Transformer models can support efficiency prediction, degradation analysis, and stability assessment. The GNN model provides strong graph-based prediction of power conversion efficiency, while the Transformer model provides useful sequential prediction of retention and degradation behavior. These findings contribute to the development of more efficient, stable, and sustainable photovoltaic technologies aligned with SDG-oriented clean energy innovation.

5. CONCLUSION

This study presented a bibliometric and physics-informed AI framework for analyzing MXene-integrated perovskite tandem solar cells. The bibliometric analysis showed rapid growth in research on perovskite tandem solar cells, indicating strong global attention to next-generation photovoltaic technologies. This trend supports the relevance of developing intelligent, stable, and efficient solar cell systems for the SDGs, particularly SDG 7 on affordable and clean energy, SDG 9 on industry, innovation, and infrastructure, and SDG 13 on climate action.

The proposed framework integrated GNNs and Transformer models using a physics-guided dataset consisting of 200 samples and 26 variables related to material composition, device architecture, environmental aging, electrical performance, defect behavior, charge transport, and stability retention. The GNN model effectively predicted photovoltaic efficiency by capturing nonlinear relationships among MXene loading, conductivity, defect density, interface quality, and power conversion efficiency. Meanwhile, the Transformer model successfully predicted retention and degradation behavior under humidity and thermal stress conditions through attention-based sequential learning.

Feature importance analysis showed that MXene loading, conductivity, defect density, interface quality, humidity, aging temperature, and testing duration were dominant factors affecting photovoltaic efficiency and stability. The hybrid physics-informed AI framework can support intelligent material optimization, degradation prediction, and long-term stability assessment of MXene-integrated perovskite tandem solar cells. This study contributes to AI-assisted photovoltaic research and provides a useful computational direction for developing efficient, durable, and SDG-oriented renewable energy technologies.

6. ACKNOWLEDGMENTS

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7. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. The authors confirmed that the paper was free of plagiarism.

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