International Journal of Engineering Research and Science & Technology

www.ijerst.org

ISSN : 2319-5991

Vol. 22 No. 1(s) (2026)

ijerst.editor@gmail.com

editor@ijerst.com

www.ijerst.com

Peer Reviewed, Referred & Indexed Journal

Research Paper

AI-Augmented Analysis of FT-IR Spectroscopy Data for Nanomaterials Characterization: A Review of Current Applications and Future Directions

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Abstract

The characterization of nanomaterials by Fourier-transform infrared (FTIR) spectroscopy generates complex, high-dimensional datasets that present significant challenges for traditional manual interpretation methods. Overlapping spectral bands, subtle chemical variations, and the need for high-throughput analysis have driven the integration of artificial intelligence (AI) and machine learning (ML) into spectroscopic workflows. This paper reviews the current state of AI applications in the analysis of FTIR data for nanomaterials. We explore how ML techniques—ranging from unsupervised learning for cluster analysis to supervised deep learning for property prediction—are being deployed to overcome the limitations of conventional chemometrics. Key applications discussed include the automated classification of graphene oxide derivatives, the analysis of nanoplastic pollutants, and the extraction of physical properties from nanoscale infrared spectra. The review also addresses critical challenges such as model interpretability, data standardization, and generalization. Finally, we outline future directions, including physics-informed neural networks, foundation models, and the development of autonomous, self-driving spectroscopic laboratories [6,7].

Keywords: Artificial Intelligence; Machine Learning; FT-IR Spectroscopy; Data; Nanomaterials;

1. Introduction

Fourier-transform infrared (FTIR) spectroscopy is a cornerstone analytical technique for the characterization of nanomaterials, offering insights into surface functional groups, chemical bonding environments, and intermolecular interactions. It is widely applied in the validation of graphene oxide oxidation states, identification of engineered nanoparticles, and detection of environmental contaminants such as micro- and nanoplastics (MNPs) [1].

Despite its analytical strength, FTIR spectral interpretation in nanomaterials research remains challenging. Spectra are often characterized by high dimensionality, overlapping absorption bands, and subtle variations influenced by synthesis protocols, sample preparation, and environmental conditions [2]. Traditional peak-picking and basic chemometric methods are frequently insufficient for resolving such complexity.

Artificial intelligence (AI) and machine learning (ML) have emerged as transformative tools in vibrational spectroscopy, enabling automated feature extraction, nonlinear pattern recognition, and predictive modeling [3,4]. By learning complex relationships within spectral datasets, AI systems facilitate automated classification, materials property prediction, and accelerated discovery workflows. This review provides a comprehensive overview of AI-enabled FTIR analysis specifically applied to nanomaterials, surveying methodologies, applications, challenges, and future prospects.

2. Rationale for AI in Nanomaterials FTIR Analysis

Conventional FTIR interpretation relies on assigning absorption bands to vibrational modes. However, nanomaterial spectra frequently exhibit broad and overlapping features, with minor spectral shifts corresponding to significant chemical differences [1]. Additionally, high-throughput materials research produces large spectral datasets that are impractical to analyze manually [4]. Machine learning offers several advantages:

- **Automated Feature Extraction:** Algorithms identify chemically significant spectral regions without subjective bias [4].
- **Advanced Pattern Recognition:** Deep learning models differentiate structurally similar materials, such as various graphene oxide derivatives, with improved accuracy [1,3].
- **High-Throughput Capability:** Once trained, models can process new spectra in real time, enabling large-scale screening [3].
- **Enhanced Analytical Sensitivity:** In nanoscale IR methods, AI assists in solving complex inverse problems to retrieve material properties beyond conventional fitting approaches [5].

These advantages justify the integration of AI into FTIR-based nanomaterials characterization.

3. AI and Machine Learning Methodologies

3.1 Unsupervised Learning

Unsupervised methods identify intrinsic structures in unlabeled spectral datasets.

- **Principal Component Analysis (PCA):** PCA reduces dimensionality while retaining maximal variance, facilitating visualization of spectral clustering trends [4].
- **Clustering Algorithms (e.g., DBSCAN, t-SNE):** Density-based clustering techniques have been applied to classify graphene oxide samples into pristine, purified, and reduced forms using ATR-FTIR spectra [1].

3.2 Supervised Learning

Supervised learning models are trained on labeled data to predict material classes or properties.

- **Support Vector Machines (SVM):** Effective for binary and multiclass spectral classification [4].
- **Random Forests:** Ensemble methods useful for polymer identification in environmental MNP analysis [2].
- **Convolutional Neural Networks (CNNs):** Particularly powerful for spectral and hyperspectral data analysis. CNNs have demonstrated success in extracting multilayer optical properties from nanospectroscopy data [3] and in polymer fingerprint classification [2,6].

3.3 Explainable AI (XAI)

Deep learning models often suffer from limited interpretability. Explainable AI tools such as SHAP and Grad-CAM help identify influential spectral regions responsible for predictions, improving chemical transparency and regulatory reliability [3,4].

4. Applications in Nanomaterials Analysis

4.1 Carbon-Based Nanomaterials

Graphene oxide (GO) exhibits structural heterogeneity due to diverse synthesis and post-treatment methods. Filatov *et al*. developed a machine learning-guided ATR-FTIR pipeline incorporating statistical analysis and clustering algorithms (e.g., DBSCAN) for automated qualitative assessment of GO dispersions [1]. Their approach successfully differentiated as-prepared, purified, and reduced GO samples solely from spectral data, demonstrating improved reproducibility over manual interpretation. This scalable methodology is extendable to other carbon nanostructures and 2D materials.

4.2 Micro- and Nanoplastics in Environmental Monitoring

Micro-FTIR (μ-FTIR) is widely used for detecting micro- and nanoplastics in environmental samples. However, spectral datasets are massive and time-intensive to process. AI-enabled workflows integrate image analysis and spectral classification to automate polymer identification [2]. Recent advancements, including AI-assisted detection platforms developed for environmental applications, have improved speed, accuracy, and standardization of MNP monitoring [6]. CNNs and ensemble classifiers significantly enhance polymer discrimination accuracy compared to conventional manual spectral matching [2].

4.3 Infrared Nanospectroscopy (Nano-FTIR)

Scattering-type scanning near-field optical microscopy (s-SNOM) extends FTIR to nanoscale spatial resolution but introduces complex tip–sample interaction physics [7].

- **CNN-Based Inversion Models:** Siebenkotten and Kästner demonstrated that CNNs can recover thin-film optical constants and thickness parameters rapidly and robustly from nanospectroscopy data, outperforming traditional iterative fitting [4].
- **Physics-Based Synthetic Data Generation:** Analytical models of s-SNOM interactions enable large-scale synthetic dataset creation for ML training, reducing dependence on costly experimental data [7].

The combination of physics-based modeling and AI offers a powerful hybrid approach for nanoscale materials characterization.

5. Challenges and Limitations

Despite significant progress, several challenges remain:

- **Data Standardization:** Lack of harmonized spectral acquisition protocols limits model generalization across laboratories [2,4].
- **Model Interpretability:** Ensuring chemically meaningful explanations for AI predictions remains critical, particularly in environmental regulation contexts [3].
- **Overfitting and Robustness:** Models trained on limited datasets may not generalize to new materials or instrument conditions [4].
- **Computational Cost:** Deep learning model training requires substantial computational resources, particularly for hyperspectral and nanoscale datasets [5].

Addressing these challenges is essential for reliable deployment of AI-driven FTIR systems.

6. Future Perspectives

The future of AI-enhanced FTIR analysis lies in increasingly autonomous and physics-aware systems.

- **Physics-Informed Neural Networks (PINNs):** By embedding vibrational and optical constraints into neural architectures, PINNs improve robustness and interpretability [4].
- **Foundation Models for Spectroscopy:** Large pre-trained, cross-modal models capable of handling IR, Raman, and NIR data could function as general spectroscopic assistants [3].
- **Self-Driving Laboratories:** Integration of robotic synthesis, automated FTIR measurement, and AI-driven decision systems could enable closed-loop materials optimization [3,4].

Such developments promise a paradigm shift toward intelligent, adaptive materials research ecosystems.

7. Conclusion

AI integration into FTIR spectroscopy represents a transformative advancement in nanomaterials characterization. Applications in graphene oxide differentiation, micro- and nanoplastic detection, and nanoscale optical property extraction demonstrate substantial improvements in automation, sensitivity, and analytical depth. Although challenges in data standardization and interpretability remain, the convergence of explainable AI, physics-informed modeling, and autonomous laboratory systems signals a future where intelligent spectroscopic platforms accelerate discovery across materials science and environmental monitoring. The synergy between vibrational spectroscopy and artificial intelligence is poised to redefine nanomaterials analysis in the coming decade.

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