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OPINION ARTICLE

Harnessing the power of machine learning in materials synthesis and characterization

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In the field of materials science, an enduring imperative exists for the investigation of pioneering materials, encompassing a diverse array ranging from graphene to shape-memory alloys, as well as bioengineered materials distinguished by their extraordinary attributes [1]. These materials hold the potential to incite transformative advancements across a broad spectrum of industries, encompassing domains as varied as electronics, healthcare, and beyond. In response to this exigent need, researchers are progressively charting a course toward a somewhat unconventional collaborator: machine learning. The harmonious convergence of machine learning and materials science has ushered in a noteworthy era marked by substantial materials synthesis and characterization advancements. This convergence portends the arrival of a promising epoch characterized by an intensified focus on innovation and the unearthing of discoveries [2].

Machine learning has brought about a transformative shift in materials science. It expedites material discovery by analyzing extensive datasets and predicting material properties based on composition and structure [3]. This streamlines the synthesis process, allowing researchers to focus on the most promising candidates and potentially unlock previously unattainable materials. Machine learning's influence extends to materials characterization, where it efficiently processes data from advanced imaging techniques, such as electron microscopy and spectroscopy [4]. It uncovers subtle features, aids in defect identification, and enhances measurement accuracy, contributing significantly to material quality control in manufacturing and our fundamental understanding of material behavior under diverse conditions [5].

From an analytical chemistry point of view, the following Table 1 depicts the application of machine learning in acquiring, comparing, confirming, and quantifying data from the following set of state-of-the-art instruments.

Machine learning can enhance the capabilities of these

Table 1. ML Applications in spectrophotometry data acquisition and analysis.

Spectroscopic technique [6-8]	Relevant library / database	Common applications of machine learning	Type of data analyzed by machine learning
Infrared Spectroscopy (IR)	NIST Chemistry WebBook, SDBS	Functional group identification, chemical property prediction, spectral resolution enhancement.	1D (Spectra)
UV-Visible Spectroscopy	SDBS, NIST UV-Vis Spectral Database	Quantitative analysis of chromophores, colorimetry real-time process monitoring.	1D (Spectra)
Nuclear Magnetic Resonance (NMR)	BMRB, NMRShiftDB	Structure elucidation, chemical shift prediction, peak picking and integration	1D (Spectra), 2D (COSY, HSQC, etc.), 3D (3D NMR)
Mass Spectrometry (MS)	NIST Mass Spectrometry Data Center, METLIN	Compound identification, quantitative analysis, deconvolution of mass spectra.	1D (Mass Spectra)
X-ray Crystallography	Cambridge Structural Database (CSD)	Crystal structure determination, parameter prediction, data processing enhancement.	3D (Crystal Structures)
Raman Spectroscopy	RRUFF Database, SDBS	Substance identification, material property prediction, noise reduction and feature enhancement.	1D (Spectra)
X-ray Photoelectron Spectroscopy (XPS)	NIST X-ray Photoelectron Spectroscopy Database	Surface analysis of materials, determining elemental composition, studying chemical states.	2D (Spectra)

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Electron Spin Resonance (ESR) Spectroscopy	ESR Database	Studying unpaired electrons in organic radicals, investigating chemical reactions, materials research.	1D (Spectra)
Mössbauer Spectroscopy	Mössbauer Effect Data Center (MEDC)	Analyzing iron-containing compounds, studying oxidation states in materials.	1D (Spectra)
Circular Dichroism (CD) Spectroscopy	CDDB (Circular Dichroism Data Bank)	Studying biomolecular structures, examining protein folding, characterizing chiral compounds.	1D (Spectra)

spectroscopic techniques by automating data analysis, improving accuracy, and providing insights that are not readily apparent through manual analysis alone. Based on the data acquired from these spectroscopic tools, machine learning can be further used for the following multi-faceted impact in materials science (Table 2).

Table 2. Examples and future aspects of ML's applications.

Application of machine learning	Example	Future Prospects in Material Synthesis and characterization
Predictive Analysis	Predicting the optimal conditions for synthesizing a bioengineered scaffold for tissue regeneration using historical data and machine learning [9]. This includes factors like scaffold composition, porosity, and growth factors required for specific tissue types.	Advancing predictive models to design and manufacture highly customized bioengineered materials for regenerative medicine, such as patient-specific scaffolds for organ transplantation and tissue repair. Machine learning can also help anticipate patient-specific responses to these materials, optimizing treatment outcomes [10].
Method Optimization	Graphene Synthesis: Machine learning optimizes precursor selection, layer control, quality enhancement, and scalability in graphene synthesis, tailoring properties for electronics and more [11]. Semiconductor Nanoparticles: ML predicts optimal conditions for size, composition, surface passivation, doping, and reaction kinetics in semiconductor nanoparticle synthesis, enhancing their performance in optoelectronics [13].	Advancing predictive models for highly customized graphene and semiconductor materials, enabling applications in electronics, energy storage, optoelectronics, and personalized healthcare. Continued optimization of synthesis processes expands their use in various industries [12].
Peak Identification	NMR in Drug Synthesis: Utilizing NMR spectroscopy for peak identification and characterization of chemical compounds during drug synthesis, ensuring product quality and purity [14].	Enhancing NMR techniques and data analysis with machine learning for faster and more accurate peak identification, advancing drug synthesis and materials discovery. Expanding NMR's applications beyond drug synthesis into diverse material synthesis processes [15].

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Data Analysis and Integration	SEM and MALDI Imaging: Employing SEM and MALDI imaging for comprehensive data analysis in material synthesis, providing insights into morphology, composition, and spatial distribution of components [16].	Integrating machine learning with SEM and MALDI data analysis to extract intricate information from large datasets, enabling precise control over material properties and advancing research in various fields, from nanotechnology to drug development [17].
Spectral Interpretation	Atomic Spectra Analysis: Utilizing spectral interpretation techniques to analyze atomic spectra, such as atomic absorption and emission spectra, to identify and quantify elemental composition in materials [18].	Advancing machine learning models for the analysis of atomic spectra, enabling real-time and highly accurate elemental analysis during material synthesis. This will play a critical role in quality control and the development of advanced materials with tailored elemental compositions [19].
Chemometric Analysis	Multivariate Analysis (e.g., PCA): Applying multivariate techniques like Principal Component Analysis (PCA) for in-depth data analysis, pattern	Further integrating PCA and other multivariate techniques with machine learning for advanced chemometric analysis. This will enable the discovery of hidden patterns in complex data,

Conclusions

The integration of machine learning represents a pivotal advancement in the quest for groundbreaking materials. Its introduction expedites the process of materials synthesis, augments characterization techniques, and extends the realm of possibility to materials previously deemed unattainable. Nevertheless, it is imperative to proceed judiciously, placing ethical considerations at the forefront of these transformative endeavors. As researchers continue to harness the capabilities of machine learning in materials synthesis and characterization, we can envisage a future marked by accelerated innovation within materials science. This rapid progress promises to catalyze advancements across a myriad of industries. The path to this promising future is illuminated by the harmonious synergy between human ingenuity and artificial intelligence, thus realizing what was once merely a dream within materials science.

Disclosure statement

No potential conflict of interest was reported by the author.

References

1. Kim E, Huang K, Saunders A, McCallum A, Ceder G, Olivetti E. Materials synthesis insights from scientific literature via text extraction and machine learning. Chem Mater. 2017;29(21):9436-9444.
2. Huang G, Guo Y, Chen Y, Nie Z. Application of machine learning in material synthesis and property prediction. Materials. 2023;16(17):5977.
3. Chibani S, Coudert FX. Machine learning approaches for the prediction of materials properties. APL Mater. 2020;8(8).
4. Moen E, Bannon D, Kudo T, Graf W, Covert M, Van Valen D. Deep learning for cellular image analysis. Nat Methods. 2019;16(12):1233-1246.
5. Kalinin SV, Ophus C, Voyles PM, Erni R, Kepaptsoglou D, Grillo V, et al. Machine learning in scanning transmission electron microscopy. Nat Rev Methods Primers. 2022;2(1):11.
6. Meza Ramirez CA, Greenop M, Ashton L, Rehman IU. Applications of machine learning in spectroscopy. Appl Spectrosc Rev. 2021;56(8-10):733-763.
7. Muto S, Shiga M. Application of machine learning techniques to electron microscopic/spectroscopic image data analysis. Microsc. 2020;69(2):110-122.v
8. Goodacre R. Explanatory analysis of spectroscopic data using machine learning of simple, interpretable rules. Vib Spectrosc. 2003;32(1):33-45.
9. Carbonell P, Radivojevic T, Garcia Martin H. Opportunities at the intersection of synthetic biology, machine learning, and automation. ACS Synth Biol. 2019;8(7):1474-1477.
10. Suwardi A, Wang F, Xue K, Han MY, Teo P, Wang P, et al. Machine learning-driven biomaterials evolution. Adv Mater. 2022;34(1):2102703.
11. Beckham JL, Wyss KM, Xie Y, McHugh EA, Li JT, Advincula PA, et al. Machine learning guided synthesis of flash graphene. Adv Mater. 2022;34(12):2106506.
12. M Dieb T, Hou Z, Tsuda K. Structure prediction of boron-doped graphene by machine learning. J Chem Phys. 2018;148(24).
13. Tao H, Wu T, Aldeghi M, Wu TC, Aspuru-Guzik A, Kumacheva E. Nanoparticle synthesis assisted by machine learning. Nat Rev Mater. 2021;6(8):701-716.
14. Fino R, Byrne R, Softley CA, Sattler M, Schneider G, Popowicz GM. Introducing the CSP Analyzer: A novel Machine Learning-based application for automated analysis of two-dimensional NMR spectra in NMR fragment-based screening. CSBJ. 2020;18:603-611.
15. Ahneman DT, Estrada JG, Lin S, Dreher SD, Doyle AG. Predicting reaction performance in C–N cross-coupling using machine learning. Science. 2018;360(6385):186-190.
16. Castro DC, Xie YR, Rubakhin SS, Romanova EV, Sweedler JV. Image-guided MALDI mass spectrometry for high-throughput single-organelle characterization. Nat Methods. 2021;18(10):1233-1238.
17. Gardner W, Winkler DA, Muir BW, Pigram PJ. Applications of multivariate analysis and unsupervised machine learning to ToF-SIMS images of organic, bioorganic, and biological systems. Biointerphases. 2022;17(2).
18. Cianciosa M, Law KJ, Martin EH, Green DL. Machine learning for

https://doi.org/10.61577/scpnmia.2024.100004

analysis of atomic spectral data. JQSRT. 2020;240:106671.
19. Michalenko JJ, Murzyn CM, Zollweg JD, Wermer L, Van Omen AJ, Clemenson MD. Machine Learning Predictions of Transition Probabilities in Atomic Spectra. Atoms. 2021;9(1):2.
20. De-la-Torre M, Zatarain O, Avila-George H, Muñoz M, Oblitas J, Lozada R, et al. Multivariate analysis and machine learning for ripeness classification of cape gooseberry fruits. Processes. 2019;7(12):928.
21. Gharsellaoui S, Mansouri M, Refaat SS, Abu-Rub H, Messaoud H. Multivariate features extraction and effective decision making using machine learning approaches. Energies. 2020;13(3):609.
22. Kunz MR, Yonge A, Fang Z, Batchu R, Medford AJ, Constales D, et al. Data driven reaction mechanism estimation via transient kinetics and machine learning. Chem Eng J. 2021;420:129610.
23. Deng W, Sha J, Xue F, Jami-Alahmadi Y, Plath K, Wohlschlegel J. High-Field Asymmetric Waveform Ion Mobility Spectrometry Interface Enhances Parallel Reaction Monitoring on an Orbitrap Mass Spectrometer. Anal Chem. 2022;94(46):15939-15947.
24. Li S, Xie RJ. Critical review-data-driven discovery of novel phosphors. ECS J Solid State Sci Technol. 2019;9(1):016013.

https://doi.org/10.61577/scpnmia.2024.100004