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Artificial Intelligence and Knowledge-Based Engineering for the Design of Environmental Nanomaterials: A Review

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Abstract

AI and KBE have been commonly applied into designing environmental nanomaterials to enhance performance, sustainability, and innovation. This review focused on how applying AI's tools such as machine learning, expert systems, predictive modeling techniques and KBE frameworks accelerates material discovery time in addition to enhancing structural design optimization and decision making for environmental applications also. Case studies illustrate applications of the computing tools to integrate experimental work in water purification, pollution control, and renewable energy. The paper makes recommendations for the revision of existing methods and new areas of investigation for intelligent adaptive and sustainable frameworks for nanomaterial design.

Keywords: *Artificial Intelligence, Knowledge-Based Engineering, Environmental Nanomaterials, Machine Learning, Environmental Remediation*

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I. INTRODUCTION

A. *Motivation for Smart Tools in Nanomaterial Design*

Significant opportunities have been presented by the progress made in nanoscience and nanotechnology to address various serious environmental issues, such as water pollutants, air pollution, soil contamination, etc. [1–2]. Nanotechnology materials such as carbon nanotubes (CNTs), metal oxides, and quantum dots (QDs) have made outstanding development for adsorbing pollutants, destructing toxic compounds, and detecting pollutants in traces. However, it remains a challenge for the design, optimization and application of these nanomaterials in practice due to their intricate and intimate relationship among various influencers such as material structure-property-environment-sustainability limitation [3].

The development of nanomaterials has historically depended on empirical testing and time-consuming simulations. With an exponentially growing number of possible nanostructure-property combinations, brute force techniques are not practical. In such a perspective, smart automated systems are highly demanded to speed up the innovation process and make it eco-efficient [4, 5]. Artificial Intelligence (AI) and Knowledge-Based Engineering (KBE) are considered to be promising approaches for addressing this knowledge gap and to provide support for data-driven decision making, generative design and rule-based automation in development of nanomaterials for environmental application [6].

B. *Scope and Objectives of the Review*

This review then aims at investigating how AI and KBE tools can transform the design and utilization of nanomaterials for environmental remediation, monitoring and sustainability. The paper initially provides explanatory description for basic concepts of AI, ML, parametric modelling, expert systems and CAD automation that is used in the further nanomaterials research. It describes the various environmental problems and disasters that demand nanomaterials and the respective designing prerequisites.

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The core of the review highlights recent advancements where AI techniques such as predictive modeling, generative design, and optimization and KBE frameworks such as rule-based systems, parametric CAD, and design automation have been successfully applied in nanomaterial design. The paper also discusses the integration of these digital tools with environmental goals, sustainability frameworks, and lifecycle considerations.

To conclude, the current review presents cross-disciplinary literature with the following objectives:

- To prove the contribution of AI and KBE in rapid, intelligent, and sustainable discovery of nanomaterials.
- To define the tools, platforms, and case studies to demonstrate the integration.
- To define the opportunities, weaknesses, gaps, and future prospects for AI and KBE as well as environmental nanotechnology.

This paper will be useful for researchers, environmental engineers, material scientists, or digital designers willing to work in cross-disciplinary teams and utilize nanotechnology for sustainable purposes.

II. Literature Review Methodology

To maximize its coverage of pertinent literature, the review followed a systematic and transparent methodology. In total, 38 separate sources were used to prepare this document: they were acquired from reputable peer-reviewed journals and conference proceedings indexed in the Scopus, Web of Science, ScienceDirect, and IEEE Xplore. Additional sources were retrieved through Google Scholar to incorporate related grey literature and newly published preprints.

The search time frame was conducted between January 2013 and June 2025. The search terms used in this review were related to studies on Artificial Intelligence, Knowledge-Based Engineering (KBE), Computer-Aided Design, and Expert Systems in nanomaterial design and environmental applications. The search terms used in this review are “AI in nanomaterials,” “knowledge-based design,” “machine learning for environmental materials,” and “CAD automation in material engineering”.

Articles were considered if they satisfied the following requirements:

- Nanomaterials and environmental materials were the focus of the study.
- AI, KBE or similar computational design methodology was applied.
- The article represented either a new evaluation methodology or its application.
- The published papers were in English and peer-reviewed.

Exclusion criteria removed papers where it was difficult to identify methodology, papers introducing methodologies not connected to the environment or design, or theoretical papers not centered on materials.

As a result of the screening of more than 188 initial records, a total of 79 studies have been reviewed and aligned to fully synthesize and analyze them. Every aligned paper has been carefully checked in terms of methodology and approach, results, and impact on the topic of AI, KBE, and design of novel nanomaterials based on them.

The general summary of the methodology will be depicted in the following Table I.

TABLE I. Methodological Overview Of The Literature Synthesis

Step	Description
Databases Searched	Scopus, Web of Science, ScienceDirect, IEEE Xplore, and Google Scholar
Timeframe	January 2013 – June 2025
Keywords Used	“Artificial Intelligence in nanomaterials,” “Knowledge-Based Engineering,” “CAD automation in materials,” “AI in environmental remediation,” “machine learning in material design”
Inclusion Criteria	Peer-reviewed journal papers and conference proceedings focusing on AI/KBE applications in nanomaterial design for environmental use
Exclusion Criteria	Non-English publications, non-peer-reviewed articles, patents, and works unrelated to environmental or materials design contexts
Initial Records Identified	~188 papers
Studies Included After Screening	79 papers
Review Method	Systematic synthesis with emphasis on comparative analysis, identification of research gaps, and proposal of future directions

The flowchart shown in the fig. 1 illustrates the sequential stages of literature identification, screening, eligibility assessment, and final inclusion of studies for qualitative synthesis in this review.

After the database search, all screened retrieved records were checked in several phases. Initially, duplicate entries were removed. Their titles and abstracts were screened to remove those not associated with environmental nanomaterials or that did not utilize AI or Knowledge-Based Engineering approaches. The remaining articles were reviewed in full text to determine their methodological relevance and whether or not they applied or contributed to the design or optimization. Only those studies fulfilling all inclusion criteria were considered in a qualitative synthesis.

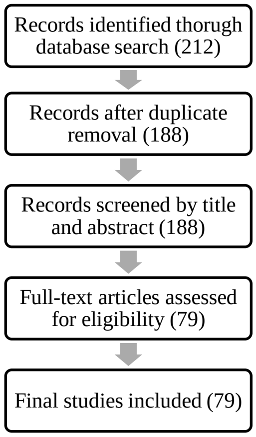

Fig. 1. Flowchart of the literature search and screening process

A formal quantitative risk of bias assessment was not performed due to this being a review addressing methodological issues and conceptual domains rather than an empirical/meta-analysis. However, potential sources of bias were acknowledged such as publication bias towards positive results and selection bias due to use of indexed; peer-reviewed databases. To reduce these, studies were considered in terms of methodological clarity; applicability to environmental applications; and coherence with recognized design principles.

III. Overview Of Artificial Intelligence And Knowledge-Based Engineering

A. Artificial Intelligence: Concepts and Relevance to Material Design

a) Artificial Intelligence (AI): It refers to the simulation of human intelligence in machines that are capable of learning, reasoning, and decision-making. Within the context of material science and environmental nanotechnology, AI plays a crucial role in identifying patterns, predicting material properties, and optimizing synthesis conditions without the need for exhaustive experimentation [7].

b) Machine Learning (ML): It is a subset of AI, enables algorithms to learn from existing datasets of nanomaterials, such as their structure, composition, and environmental performance, and make accurate predictions for new, untested materials. Supervised learning (such as support vector machines, decision trees, and neural networks) is widely used for classification and regression, such as predicting band gaps, surface area, or adsorption performance [8]. Unsupervised learning would be used to cluster materials, or to discover hidden correlations in large material databases [9].

c) Deep learning: By means of artificial neural networks and convolutional frameworks, deep learning has gained popularity in modeling nonlinear relations of high-dimensional data of nanostructural systems. Such AI tools could substantially speed up the material discovery cycle and decrease the cost of development [10].

B. Knowledge-Based Engineering (KBE): Principles and Application

KBE is a systematized approach for the incorporation of the knowledge of domain-specific rules, logic and heuristics into computer-aided systems to automate and guide engineering design activities [11, 12]. KBE systems encode expert experience as rules, ontologies, decision trees, and templates, serving as a basis for a consistent, repeatable, and intelligent design-to-operation process [13, 14].

In the domain of nanomaterials, KBE can assist in:

- Selecting appropriate materials based on environmental requirements (e.g., selecting nanomaterials with high photocatalytic activity for water purification) [15].
- Guiding synthesis parameter choices using encoded expert rules [16].
- Automating the layout and testing workflows within CAD environments [17].

KBE extends traditional CAD by embedding knowledge into design models, allowing for automatic updates and design regeneration when parameters change [11]. This is useful for mapping bulk-sensitive materials such as nanostructured surfaces, coatings, or device geometries at different design iterations.

C. Parametric Modeling and Expert Systems

Parametric models provide the possibility to generate adaptive digital models in which geometry and underlying behavior are controlled through parameter manipulation [18]. In the field of environmental nanotechnology, such bricks are very helpful in modeling nanoporous materials, multilayer membranes or surface-coated particles. Design parameter variation (e.g. pore size, layer thickness and material composition) can be directly included in the digital model, enabling efficient simulations and optimisations [18, 19].

Expert systems, on the other hand, are rule-based reasoning tools that emulate the decision-making abilities of human experts [20]. They are particularly advantageous in the early design screening as they can screen a set of feasible nanomaterial candidates applicable for given environmental conditions, such as pH, pollutant type or rate of flow. When combined with AI algorithms, expert systems transform into hybrid intelligent systems which can reason, learn, and adapt dynamically [21].

D. Integration with CAD Tools and Automation Platforms

AI and KBE have been interfaced with CAD systems for automated creation of nanomaterials geometries, mesh-able structures for simulations, and interfaces to multiphysics simulation (CFD or MD or optical) [22]. Contemporary CAD systems use scripting (e.g., Python or MATLAB APIs) to provide AI and KBE rules a control of the geometry generation process [23, 24].

For instance, AI-based generative design may recommend novel shapes of nanostructure that achieves a maximum surface area for filtration membrane with minimal pressure drop.

Meanwhile, KBE systems could evaluate such arrangements regarding the manufacturability, cost and sustainability [25].

These capabilities are further extended by automation platforms which combine databases, simulation tools, and performance evaluators to form a close-loop design environment for shaping the rapid environmental nanomaterial innovation [26]. The Conceptual framework of AI and Knowledge-Based Engineering components relevant to nanomaterial design is shown in the fig 2. Fig. 2 is the author-created schematic emphasizes the synergistic relationships of AI methods (e.g., machine learning, deep learning, expert systems) and KBE components (e.g., rule-based reasoning, parametric modeling, CAD integration). This figure shows how we predict with products catalog data and decide on policy knowledge then lead to an intelligent and sustainable environmental nanomaterial design.

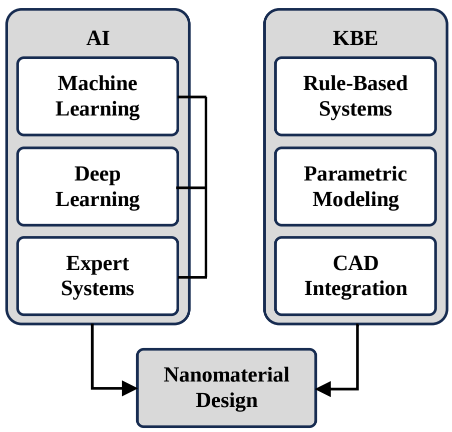

Fig. 2. Conceptual framework illustrating the interaction between Artificial Intelligence (AI) and Knowledge-Based Engineering (KBE) in nanomaterial design

IV. Environmental Nanomaterials: Design Needs And Applications

A. Common Nanomaterials Used in Environmental Remediation

The unique physical, chemical, and structural properties of nanomaterials are utilized to remediate pollution and develop sustainable techniques in environmental nanotechnology. Material at the nano-size scale has a high surface area-to-volume ratio, quantum size effects, and high reactivity, so it would be suitable for environmental applications. Many types of nanomaterials have been extensively studied and applied, including:

1) Metal Oxide Nanoparticles: Titanium dioxide (TiO_2), zinc oxide (ZnO), and iron oxide (Fe_3O_4) are widely used for photocatalysis, pollutant degradation, and heavy metal removal due to their optical and magnetic properties [27].

2) Carbon-Based Nanomaterials: As synthesizable materials with tunable porous structure and excellent electrical conductivity, both Carbon nanotubes (CNTs), graphene and activated carbon nanosheets could be readily applied as promising adsorbents for both filtration and sensing [28].

3) Zero-Valent Metal Nanoparticles (nZVI): The high redox potential of zero-valent iron and silver nanoparticles is well established due to its capability to degrade organics pollutants and in microbial disinfection [29].

4) Metal – Organic Frameworks (MOFs): These hybrid crystalline materials with a high specific surface area and functional groups, are ideal for gas separation and environmental sensing applications [30].

These materials are often produced with surface treatments, composite formulations or multiscale structures to enhance their environmental performance.

B. Key Application Areas

Environmentally Sustainable Nanomaterials play a critical role in achieving environmental sustainability. Their applications can be categorized in three major components: Pollution control, Resource recovery and Real-time environmental monitoring.

1) Water Purification: Nanomaterials are used as part of membranes, filters or adsorbents to eliminate diverse pollutants such as heavy metals, organic dyes, pharmaceuticals and microorganisms. Photocatalytic nanoparticles, e.g., Titanium dioxide (TiO2), decompose organic pollutants under UV or visible light, and CNTs and graphene materials are characterized by high adsorption capacities [31].

2) Air Filtration and Gas Treatment: Filters and coatings of nanostructured materials are employed to mitigate the release of fine particles (PM2. 5 and PM10), reactive gases, volatile organic compounds (VOCs) and greenhouse gases. Functionalized nanoparticles can improve catalytic NOx, SOx and CO_2 emissions abatement from both industrial and motor vehicles [32].

3) Soil Remediation: Nanoparticles can fix or decompose soil contaminants by redox reactions or adsorption. For instance, to remediate chlorinated solvents use of nZVI particles and for stabilization of heavy metals use of nanoclays [33].

4) Environmental Sensing and Monitoring: The nanosensor have a good sensitivity and excellent selectivity for monitoring of pollutants including arsenic, nitrates and gases at trace level. Surface-enhanced Raman spectroscopy (SERS), QDs, and nanoelectrodes are the three types of intelligent environmental monitoring systems [34].

The design needs and related applications of different environmental nanomaterials are shown in Fig. 3. This figure, proposed by the authors, classifies key classes of environmental nanomaterials metal oxides, carbon-based nanomaterials and hybrid composites based on their main application field ranging from water purification to air filtration up to soil remediation platforms, as well as in environmental sensing and clean energy counterparts.

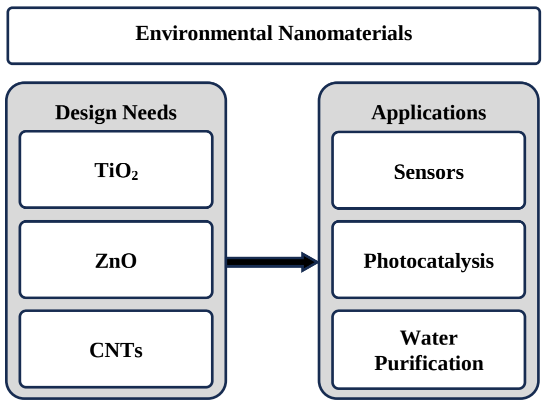

Fig. 3. Classification of environmental nanomaterials and their application domains

C. Challenges in Conventional Design Approaches

While they hold great potential, it is challenging to rationally design nanomaterials for environmental uses for a few reasons:

1) Multifunctionality and Trade-Offs: A material may possess good adsorption but not good photocatalytic activity and/or it might be highly unstable in the environment. On the other hand, it is difficult to meet multiple performance targets in the conventional CAD flow [35].

2) Material Combinatorics: There are too many combinations, morphologies and functionalization of surfaces for exhaustive experimental investigation [36].

3) Environmental Constraints: The selected materials have to perform in different environmental conditions (e.g., pH, temperature, ionic strength) and based on the environmental regulations (safety, regulation of sustainability) [37].

4) Scale-Up and Reproducibility: Many laboratory-scale nanomaterials are highly promising but not successfully scaled up because of complexity in synthesis or low or varying performance [38].

These are challenges that exact the demand for intelligent, automatic and adaptive design tools where AI and KBEs could indeed be a revolution.

D. Critical Commentary on Environmental Nanomaterials

There are several reports on TiO_2 and ZnO nanomaterials application for PCP, but most of them are limited to the laboratory scale studies under UV source. As a result, the understanding regarding their behaviors under solar or indoor light is precluded. In contrast, carbonaceous nanomaterials have orders of magnitude higher adsorption capacity and are still underutilized in terms of their long-term stability and reusability. To overcome these limitations, not only a step toward new material synthesis but also an approach from predictive modeling with AI is required to search for the sub-optimal material-environment combination.

V. Applications of AI and KBE in Nanomaterial Design

AI and KBE, was also applied for designing nanomaterials to solve environmental problems, fundamentally changing the fabrication, testing and optimization of materials [4]. These tools support more informed decision-making, reduce manual intervention, and enable efficient analysis and implementation.

A. AI for Predicting Nanomaterial Properties and Behavior

AI is very convenient to study and predict the multiscale behavior of nanomaterials in various environments, especially for ML. Using the characterization results and available experimental data, as well as computer simulated information, ML models can predict critical properties like surface area, porosity [39], bandgap energy, photo-catalytic activity [40], adsorption capacity and selectivity [41], environmental stability and toxicity [42].

For example, supervised learning techniques like support vector machines (SVM), random forests or neural networks have been applied to forecast the adsorption properties, in wastewater treatment, of carbon nanomaterials and metal oxides [42].

In addition, deep learning models can describe complex structure property relationships such as details about how nanoparticle morphology affects the decay rate of pollutants. These predictive capabilities minimize the use of trial-and-error and enable virtual screening of thousands of candidate materials prior to experimental synthesis [43].

B. KBE for Rule-Based Design and Material Selection

KBE systems, which are used to capture expert knowledge, design rules and environmental constraints in the form of reusable templates or logic structures. For instance, KBE enables picking materials having pre-determined properties (e.g., non-toxicity, recyclability or surface activity) in environmental nanomaterial design [44], automates the development of hierarchical nanomaterials (e.g., multilayer membranes, coated nanoparticles) [45] and facilitates evaluation guidelines for environmental policies and sustainability [46].

The KBE system could generate some core-shell material advice for the degradation of certain pollutants in photocatalysis by some specific core-shell materials on the basis of laws from a nano-material database with corresponding rules [47]. These systems can help reduce design variance between teams or projects and increase reproducibility.

C. CAD and Automation for Rapid Prototyping

CAD is also essential in linking the concept to real nanomaterial synthesis. Classical CAD tools are good for geometric modelling, visualization but weak to model complex nano-scale architectures or encode heuristic domain knowledge. The recent innovations in CAD have further enhanced its functionality by integrating rulebased modeling and simulation driven design, where the preliminary performance estimations are done prior to the actual fabrication [48, 49].

The blending of AI and KBE in CAD will transform CAD from a passive modeling to an active, knowledge-based design system. AI brings with it predictive modelling, automated optimization and generative design functionality that complement KBE's capability to retain expert rules, constraints and best practice templates for material selection and configuration. In combination, these features facilitate the generation of fast design alternatives, multi-criteria (performance, cost, sustainability) evaluation and sharing domain knowledge between iterative sections of the design timeline.

For example, hybrid CAD–AI workflows for membrane design where pore geometries are generated that optimize flux while automatically accommodating selectivity and CAD coupled with KBE knowledge bases which maintain project manufacturability and environmental criteria during geometry generation. Quite crucially, this integration also enables a closed-feedback loop: CAD geometries are used to drive simulations (e.g., CFD, optical models, mechanical analysis), results inform the evaluation of AI/KBE and optimal solutions are looped back into CAD for design enhancements.

Fig. 4 is a workflow diagram showing how AI and KBE tools assist in nanomaterial design from data input, rule-based modeling, simulation, to material selection. This author-created workflow diagram gives an overview of the flow. The diagram highlights the loop of AI and KBE for automated design, optimization, and decision-making towards environmental nanomaterials.

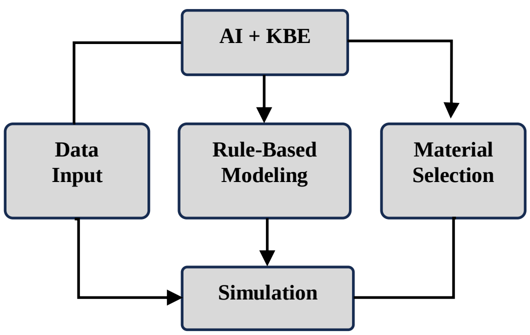

Fig. 4. Workflow illustrating the integration of AI and Knowledge-Based Engineering in nanomaterial design and optimization

Based on the CAD-assisted, AI–KBE-integrated design framework as introduced above, the following subsection summarizes and critiques recent studies that adopt these approaches (i.e. their methodology, benefits and limitations) so that lessons may be drawn to guide future research.

The contrastive synthesis of AI with KBE in the nanomaterial design problems from both strengths and limits aspects is summarized in Table 2 to make clear their respective roles and synergies.

TABLE II. COMPARATIVE ROLES OF AI AND KBE IN ENVIRONMENTAL NANOMATERIAL DESIGN

Aspect	Artificial Intelligence (AI)	Knowledge-Based Engineering (KBE)
Core principle	Data-driven learning and pattern recognition	Rule-based reasoning using expert knowledge
Primary function	Property prediction, optimization, pattern discovery	Design automation, decision logic, consistency
Data dependency	Requires large, high-quality datasets	Relies on structured domain knowledge
Interpretability	Often limited (black-box models)	High (explicit rules and logic)
Adaptability	High adaptability with new data	Limited adaptability without rule updates
Design automation	Indirect (via optimization algorithms)	Direct (rule-driven CAD automation)
Typical applications	Predicting adsorption efficiency, catalytic activity	Material selection, parametric model generation
Limitations	Data bias, limited explainability	Knowledge acquisition and maintenance effort
Complementary role	Provides predictive intelligence	Provides traceability and design control

D. Recent studies with AI and KBE

Recent studies applying AI and Knowledge-Based Engineering (KBE) in environmental nanomaterial design differ significantly in terms of methodology, data dependency, and degree of automation [50-52]. Machine learning–based approaches predominantly emphasize property prediction and process optimization, offering high computational efficiency but often relying on limited or domain-specific datasets, which constrains generalizability. In contrast, KBE-driven studies focus on rule-based material selection and design consistency, enabling repeatable and transparent workflows, but they lack adaptability when new material classes or experimental data emerge [53-55]. Hybrid AI–KBE approaches attempt to bridge these gaps by combining data-driven prediction with expert knowledge, improving interpretability and decision traceability. However, most hybrid frameworks remain validated only at laboratory scale and face integration challenges related to data standardization, software interoperability, and knowledge base maintenance [56-59]. Comparative analysis across these studies reveals that no single methodology sufficiently balances accuracy, interpretability, scalability, and sustainability, underscoring the necessity for integrated design frameworks [60].

Table 3 shows the comparison overview of major studies seeded for environmental nanomaterials implementation using AI and KBE methods.

TABLE III. KEY STUDIES COMPARING AI AND KBE IN ENVIRONMENTAL NANOMATERIAL DESIGN

Authors	Methodology	Main findings	Limitations
Konstantopoulos et al. [55]	Use of AI-driven predictive modeling and machine learning (including Bayesian networks) for materials discovery, property prediction, and impact assessment. Reliance on standardized, curated data for accurate predictions. Implementation of ontology-assisted co-simulation and cognitive digital twins for real-time monitoring and	Machine learning speeds materials development from 10 to 20 years to about 18 months, helps with nanoengineering problems such as modeling pulse electrodeposition, and identifies process design trends for new therapies and safe bio-nanomaterials	The limited access to failed results and reproducibility are the main challenges. Conventional material discovery is difficult because of the long time to market and low scalability.

Authors	Methodology	Main findings	Limitations
	performance forecasting. Strategic guidance from EMMC and Nanoinformatics Roadmap 2030.		
(Naik & Jagtap [61]	The study reviews existing literature on AI–nanotechnology integration, highlighting their synergy, challenges, opportunities, and future prospects	The review highlights the synergy between AI and nanotechnology, where machine learning, deep learning, and neural networks enhance efficiency, precision, and scalability, enabling transformative advancements across domains	Not mentioned (the abstract does not specify any limitations)
Mutha et. al. [56]	The methodology reviews literature on AI in nanomanufacturing, focusing on machine- and deep-learning for material synthesis, process optimization, and quality assurance, while discussing challenges like data availability, security, and complexity, and summarizing AI algorithm applications.	AI for nanomanufacturing enables new material synthesis, process optimization and characterization. Both machine- and deep-learning methods are troubled in some regards, but newer techniques such as reinforcement learning or XAI show potential. Nanoparticle synthesis and semiconductor fabrication have also been revolutionized by AI, with the possibility for additional optimization in efficiency, quality and sustainability	Challenges express themselves in terms of data limitations, lack of transparency, complexity as well as variability of material properties. Additional issues: security and privacy, training and integration, technical restrictions, compliance requirements, incompatibility with the equipment and higher prices
Chen et. al. [52]	The study reviews recent AI applications in nanomaterials discovery, outlines limitations and challenges, and highlights future research directions.	AI is also hastening the discovery of nanomaterials that underpin clean energy and carbon capture technologies. In addition, recent progress involves solar cells, hydrogen energy, battery and CO_2 capture materials. In this review, the current challenges are discussed, and perspectives of future research directions for massive AI integration are presented.	Not mentioned (the abstract does not specify the limitations or challenges)
Singh et al., [62]	Use of AI/ML techniques, including PBPK and nano-QSAR models, high-content image-based screening, and advanced algorithms for diverse data analysis and validation	Safe medical use of nanomaterials requires thorough nanotoxicology. AI/ML techniques like PBPK and nano-QSAR predict behavior and toxicity, though model reliability is challenged by complexity, variability, and limited high-quality data	Challenges are the poor knowledge of chemical mechanisms and toxicity, inconstant preclinical testing, risk of ML overfitting, paucity of high-quality data, nonstandardized nanomaterial description and dynamic nanoparticle environment interactions.
Ur Rehman et al. [53]	Literature review advocates AI/ML in nanotechnology, using EfficientNet-B7 with pyramidal attention and dilated convolutions for multiscale feature extraction. Implemented on a high-performance PyTorch system with Python libraries for data handling and visualization, focusing on attention-over-attention networks for retinal disease recognition	The deep learning network had an accuracy rate of 98.74% in identifying those with retinal diseases based on OCT images. Novel attention mechanisms and multiscale features can also boost the performance of subtle anomaly detection. Ablation studies verified the design, and demonstrated the necessity of every part.	Limitations include single-scale feature extraction, weak attention mechanisms, and limited contextual capture. Challenges involve complex retinal structures, need for refined attention, additional datasets, and balancing performance with complexity
Han et al., [63]	Focus on hardware design, software optimization, AI-enabled process control, and case studies on quantum dots and gold nanoparticles.	The review explores automated synthesis strategies for inorganic nanomaterials, showing improved efficiency via closed-loop systems and ML-enabled optimization, and emphasizes	Challenges include poor batch stability, scaling issues, complex quality control, cross-scale modeling, high-throughput integration, and developing standardized databases.

Authors	Methodology	Main findings	Limitations
		automation, intelligent technologies, and human–machine collaboration in understanding synthesis mechanisms.	
Wang et al., [64]	Use of ML for data analysis and bibliometrics, performing systematic, multidimensional analysis of scientific literature and diversified ML applications.	This review first quantitatively discusses ML-guided nanomaterial design and then interprets the applications, key ML algorithms used, current challenges and future directions from three aspects: data quality, algorithm innovation and interdisciplinary penetration.	Key focus areas limited to data quality and dataset construction, algorithm innovation and optimization, and strengthening interdisciplinary collaboration.
Yan et al. [65]	AI and molecular simulations tools transform nanotoxicity data into actionable public health information include the development of quantitative structure–toxicity relationships, understanding the mechanistic underpinning of toxic phenomena, constructing model-friendly databases, using state-of-the-art nanodescriptors for simulation studies, implementing new approaches in modeling etc., and facilitating the design of next-generation nanomaterials	AI and molecular simulation transform nanotoxicity data into quantitative structure–toxicity relationships, and uncover molecular mechanisms. The review emphasizes the current unmet needs and tools such as model-friendly databases and predictive nanodescriptors. It presents future directions and challenges of AI- and simulation-based nanotoxicology research.	Challenges include limited high-quality nanomaterials, non-standardized nanotoxicity data, lack of model-friendly databases, scarce universal nanodescriptors, and difficulty simulating nanomaterials at realistic scales.
Badini et. al. [4]	Integration of AI/ML for predicting material properties and designing new materials through a materials informatics (MI) framework, covering data acquisition, representation, mining, multi-modal integration, physics-based deep	AI is transforming materials design by predicting properties, enabling new materials with enhanced features, streamlining discovery, and supporting mechanical property predictions.	Core AI/ML success depends on the availability of high-quality, labeled data, but models hit generalization limits and struggle to fold in physics and causality across high-dimensional or
	learning, materiomics, computer vision, transfer learning, and autonomous material discovery.		dynamic simulations. The resulting limited capacity for designing novel solutions (e.g., proteins) hinders the broader application and multiscale integration of AI.
Salaza et al. [1]	Review of nanomaterials (noble metals, biosensors, cyclodextrin polymers, graphene oxide) for the detection and remediation (photodegradation, wastewater treatment) of heavy metals and agrochemicals.	Nanomaterials (due to their unique properties) are critical, sustainable alternatives for pollutant detection and remediation, emphasizing reusability and specificity. Key challenges remain in scaling up nanomaterial synthesis and developing effective recovery/reuse procedures.	Scaling up synthesis requires greener, low-cost methods, and establishing effective recovery and reuse procedures to meet sustainability goals and reduce costs. Future studies should aim to clarify the potential toxicities and long-term effects on environment, surpass the drawbacks which are associated with lab-scale procedures and critically analyze for possible interferences in real matrices.
Salem et al. [66]	Synthesis Methods: Nanomaterials are produced via Physical (deposition, lithography, milling, aerosol), Chemical (coprecipitation, hydrothermal, electrochemical), and Biological (fungi, algae, bacteria, yeast mediated) routes. Characterization Techniques: Analytical confirmation uses techniques like Spectroscopy (UV-Vis, FTIR, XRF)	This review provides an in depth introduction of types of nanomaterials, their synthesis and applications (environmental/biomedical), representing where technology finds its potential utilization. It also contrasts synthetic vs. natural nanoparticles to recognize and adjust the gaps of knowledge for	Synthesis Challenges: Production (particularly bottom-up) is hindered by cost, toxic side products, difficulty in scaling up, limited diversity of biological approaches, and the difficulty of predicting the novel properties of unique nanoparticles often synthesized far

Authors	Methodology	Main findings	Limitations
	and Microscopy (TEM, SEM), along with Zeta Potential Analysis.	environmental use.	from equilibrium. Challenges in Application: The uneven dispersion of technical catalysts, short duration (due to the weak leaching/degradation resistance), and a more extensive application for water treatment etc., stimulate further exploration to mechanisms such as antibacterial activity on metal-oxide nanoparticles.
Asghar et al. [67]	A systematic literature review on nanomaterials for environmental remediation was conducted. Bibliometric analysis was performed using SCI data, VOS viewer, and CiteSpace 5 (co-citation analysis) to map research networks, identify hot topics, and track current trends.	Nanomaterials (NMs) provide cost-effective and sustainable solutions to the upgrading of pollution management, showing great potential in efficient contaminant remediation. The research focus on NMs for air and water treatment has been raised remarkably (from 2013 to 2022) corresponding with the promises that they display in environmental control	Nanomaterials (NMs) and advanced materials such as MOFs/NCMs (Nickel-Cobalt-Manganese) are confronted with several main challenges, including expensive costs, reduced stability/durability, poor selectivity/adsorption capacity and recycling difficulties. In the future, special attention should be paid to emerging avenues of synthesis for better dispersibility, retention ability and scale up as well as cost-efficient preparation of NMs and provide a full account on their potential toxicity and safety and possible adverse effects toward the
			human health and environment
Serov & Vinogradov [68]	Reviewing data-driven approaches, high-throughput experimentation (HTE), automation, AI, and ML for designing and optimizing drug delivery systems (DDSs) and related nanomaterials	Drug Delivery Systems (DDSs), in particular, nanomedicines have shown great improvement for pharmaceutical products, but there are still challenges associated with their rational design and the high-throughput discovery due to complications of data. Development of efficient nanoformulated drugs and smart materials calls for combining data science, HTE, automation, AI, and ML	The rational design and high-throughput optimization of nanomaterial-based DDSs remain immature as scientists do not have sufficient ability to retrieve, analyze, store and manage the multidimensional data
Miller et al. [69]	Methodology involved systematic searching, selection, and subsequent thematic, comparative, and meta-analysis of relevant studies.	The combination of AI and IoT has revolutionized the field of environmental monitoring with superior, precision data collection and analytics. This collaboration provides strong advantages such as increased data accuracy, low costs, scalability of operations and proactive management services if the impediments are overcome, mention data security and data quality.	The main challenges include issues related to data quality, interoperability, security, technical constraints, and ethical concerns.
Satyam & Patra [70]	Research focuses on nanotechnology to develop new adsorbent materials, with AI/ML and theoretical/kinetic models used for process optimization and predicting behavior.	In this paper, the idea of how these new materials can reshape our sustainable criteria for water purification and follow green chemistry concepts is addressed.	Technical difficulties are restricting the effectiveness of adsorbents in these applications, such as low capacity, poor selectivity, stability/fate degradation and

Authors	Methodology	Main findings	Limitations
	Analytical techniques (SEM, HPLC) and molecular simulations (DFT) are used to understand mechanisms, while integration with membranes enhances recovery and reusability.	Solving the challenge on a large scale necessitate a cross-disciplinary approach to breaking the existing barriers and adopt emerging technologies	difficulty in recovery/reusability. More general obstacles comprise the high costs of production/regeneration including potential environmental/ health risks associated with nanomaterials as well as a (still) absent, standardised regulation and guidance.
Liu et al. [71]	Methodology: A comprehensive literature review focusing on fundamental machine learning techniques and recent AI advancements in materials science for energy storage.	Artificial intelligence has emerged driving innovation in materials science for electrochemical energy storage (batteries, fuel cells, and supercapacitors), and is dramatically shortening the discovery period of next generation materials. The paper also gives an overview of the potential offered by AI to improve performance, durability and safety, as well as unlock new research frontiers in the field industry	Not mentioned (the abstract does not provide any specific limitations or self-reported problems)
Alaneme et al. [72]	Systematic literature search and critical review of studies on AI techniques (ML algorithms, optimization models) in geopolymer-concrete production. Analysis focused on benefits, challenges, research methodologies, and findings related to using AI for optimizing mix design, curing, and material selection	This review demonstrates the benefits and challenges of using AI techniques (specifically for optimizing mix design, curing, and material selection) in geopolymer-concrete production. The application of AI aims to improve sustainability and performance, offering significant practical implications for industry professionals	Key challenges include limited data availability, high computational complexity, and difficulty in integration and practical implementation within existing production processes, necessitating further research.
Narsimha Mamidi et al. [73]	This comprehensive review systematically surveys metallic and nonmetallic nanomaterials, focusing on methodical design principles and recent advancements across diverse applications.	Nanocomposites are emerging as key, versatile players in healthcare, energy storage, and environmental remediation due to their simplicity, lightweight, and cost-effectiveness. Despite promising clinical and translational applications demonstrated by current research, challenges persist in their development and widespread application.	Not mentioned (the abstract does not specify the limitations or challenges)
Papadimitriou et al. [74]	AI methodologies reviewed include Materials Informatics, Active Learning, Self-Correcting Processing, and Digital Twins. These leverage computational techniques like Density Functional Theory (DFT), Molecular Dynamics, and Finite Element Analysis (FEA), with consideration for big data and data quality.	This review provides an overview of AI approaches (Materials Informatics, Active Learning, Digital Twins) and computational tools (DFT, MD, FEA) for materials design as well as discovery. In smart manfacturing, AI is bringing a sea-change by fine-tuning rather than pursuing process excellence and ingesting big data / quality for self-quality and self-correcting.	Not mentioned (the abstract does not specify any limitations or challenges)
Bibri et al. [75]	The study employs a comprehensive systematic review methodology using a unified evidence synthesis framework that integrates aggregative,	The research contributes to advancing knowledge about the promise of AI and Artificial Intelligence of Things (AIoT) technologies for	A significant gap exists in understanding the smarter eco-cities paradigm and the challenges/barriers in implementing

Authors	Methodology	Main findings	Limitations
	configurative, and narrative approaches.	promoting a sustainable urban environment, as well as recognizing the challenges involved in realizing that promise. These results are informative and they give perspective so as to enable decision-makers towards priorities on environment well-being	AI and AIoT solutions.
Popescu et al. [76]	Methodology: Systematic review via literature search using AI, IoT, and environmental monitoring keywords, followed by visualization and synthesis of results using VOS viewer software.	Sensors based on AI and advanced technologies' integration appear as a promising alternative for in-line environmental monitoring, meaning an important contribution to the identification and prevention of hazardous substances (in soil, plants, waste). Such systems ensure food crop safety, environmental protection and in turn preclude human exposure by means of real-time detection, localization tracking, predictive modeling, risk assessment of harmful materials	Technical and Economic Barriers: Constraints include model performance / interpretability tradeoffs, high computational energy costs, infrastructure constraints (e.g., in developing countries), and high data capture (precision ag). Implementation and Societal Considerations: There exist major challenges regarding the sharing, ownership, privacy, cyber security of data; resistance to adoption (job concerns), lack of expertise in AEC (Architecture, Engineering, and Construction) industry, and also difficulties on understanding AI in decision making.
Kumah et al. [77]	A scoping review of literature (June-July 2021) on nanoparticle effects on health/environment was conducted	This scoping review examines nanoparticles' toxic effects on human health (cell death, DNA damage,	Methodological restrictions were that the review was limited to English language

Authors	Methodology	Main findings	Limitations
	following JBI and PRISMA guidelines. The methodology involved a two-step screening process, data extraction using Covidence, and analysis via narrative synthesis.	inflammation, etc.). It highlights a significant gap in research concerning the environmental impact of nanoparticles.	studies since 2000 and significant underrepresentation of comparative data on immortalized vs. primary cell lines as biomarkers. It also showed limitations of knowledge regarding the environmental effects of nanoparticles (and in particular for certain materials like Platinum, Gold, Magnesium Oxide, Molybdenum/Tungsten trioxide and Carbon Black) and their specific toxic effects
Dharmalingam et al. [78]	Development and outlining of essential, novel, sustainable, and environmentally friendly (including green) synthesis procedures for metal oxide/sulfide-based nanocomposites.	Green technologies are essential to fabricate metal oxide/sulfide based nanocompositions for efficient decontamination of organic dyes through photocatalysis. These multifunctional nanocomposites exhibit pristine properties that can be utilized in various fields, including energy storage, antimicrobial activity and heavy metal detection which have great future prospects for research	There is enormous scope and need for future research and application to address current limitations and further investigate this area.

Overall, evidence for comparison suggests that hybrid AI–KBE systems offer the greatest potential route toward environmental nanomaterial design, provided issues concerning data quality and integration of valid data sources are resolved systematically.

1) Water Purification and Wastewater Treatment: Many works have used AI and KBE methods to the design of water-cleaning-related nanomaterials. Machine learning models have been extensively applied to predict adsorption capacity, membrane permeability and fouling behavior, while KBE approaches supported material selection and parametric design of Filtration membranes. Such methods work well under limited (controlled) dataset and application specific scenarios, showing their difficulty in scaling up to real world applications.

2) Air Filtration and Pollution Control: Artificially intelligent optimization has been applied in air filtration and pollution treatment to create nanostructured filters, and catalytic materials for cleansing particulate matter including gaseous pollutants. In contrast to water treatment investigations, where flow dynamics and surface reactivity normally take the highest priority, air-oriented applications are mainly solving laboratory testing procedures. However, the integration of KBE in this field is limited, mainly concentrating on individual predictive modeling without addressing automated design process.

3) Soil Remediation: Applications of AI and KBE to soil remediation mainly target the prediction of contaminant–nanomaterial interactions and identification of optimal nanoparticles for in situ treatment purposes. Although prediction precision is encouraging, the majority of reported studies are not yet validated in long run or applied at field scale so that their practical use is minimal.

4) Environmental Nanosensing: AI related methods have been widely utilized in designing of the nanosensors for environmental monitoring, heavy metal and toxic gas detection etc. Deep learning algorithms enhance the sensitivity and selectivity, while KBE is good at rule-based sensor deployment. These platforms possess high analytical performance, but still suffer from problems of sensor stability and data reliability.

5) Clean Energy and Sustainable Environmental Systems: For clean energy, AI and KBE have been applied to the design of nanomaterials in photocatalysis, energy storage and hydrogen generation. In comparison with remediation-based research, when it comes to energy applications multi-objective consideration of efficiency, cost and sustainability is important. Although encouraging successes have been realized, most methods are still computationally oriented, and their experimental integration is limited.

E. Knowledge Gaps

Although substantial progress has been achieved, there are still some missing pieces in the existing usage of AI and KBE at environmental nanomaterial design. The current studies usually consider prediction by AI techniques and reasoning based on KBE independently which causes a broken workflow. Besides, few common datasets and weak experimental verification have had negative impacts on the applicability of existing models. The lack of consolidated systems containing design automation, performance assessment and sustainability evaluation reveals an important void which needs to be addressed in order to ensure robustness and scalability.

VI. Challenges And Future Directions

Although AI and KBE have demonstrated tremendous promises in environmental nanomaterials design, several outstanding issues remain to be resolved before the full potential can be realized. These are technical, data challenges, environmental issues and support integration. At the same time, the field presents several exciting opportunities for future exploration and development.

A. Key Challenges

1) Data Availability and Quality: One of the primary barriers to effective AI-driven nanomaterial design is the lack of comprehensive, standardized, and high-quality datasets. Experimentalists' data is frequently distributed over many publications and inconsistent in style, or it completely lacks the necessary descriptors. Industrial data sets are often not accessible due to proprietary restrictions. In the absence of large and diverse datasets, a machine learning model may be overfit (driven by noise) leading it to draw incorrect conclusions or generalize poorly when presented with new unseen instances, or more generally that such models will give improper relations for physical effects.

2) Model Interpretability and Trust: Most AI models, particularly deep learning networks, are referred to as “black boxes” because they are not easy to interpret. In high-stakes environmental applications, designers, regulators, and engineers must have confidence in the AI-based recommendations or predictions and understand the basis for them. Explainable AI (XAI) technologies are in its infancy in materials science and need further refinement to reach reliable and acceptable standards.

3) Integration Bottlenecks: There are practical issues in integrating AI, KBE and CAD systems despite their conceptual concurrence. Data silos, software interfaces that do not speak to each other and missing communication protocols are just a few roadblocks that prevent an optimized process. Further, many environmental scientists may not have the technical expertise to adequately modify and implement AI–KBE systems.

4) Sustainability, Safety, and Ethical Concerns: AI application in material design should be done based on principles of green chemistry, eco-efficiency and life cycle sustainability. However, current AI-KBE tools seldom incorporate modules enabling the environmental risks, materials toxicity and end-of-life consequences. Focus is also shifting to the ethics of AI bias, as well as over-automation and the obsolescence of traditional skills in materials development.

B. Critical Evaluation and Implications

AI-based KBE for nanomaterial design is a game-changer in the history of computational materials. However, a summary of the earlier studies is required to reveal the underlying issues and constraints that require further investigation.

The first issue is that there is a lot of really good work in the predictive modeling or optimization realms but fewer validations with experimental data. The reliance on the virtual data beyond this point, which is synthetic in nature, makes it inconvenient to apply knowledge and understanding learnt from AI-based models to practical work and raises a gulf between computational insight versus bench-side investigation. And even though KBE systems have worked great for rule-based material design and robotics applications, these mainly consist of static knowledge bases that have to be regularly updated in order to keep up with the latest advancements in fast developing fields like nanotechnology.

The second issue is interdisciplinary integration remains limited. AI algorithms are also rarely directly embedded within the CAD environment or connected to existing materials databases, therefore workflows tend to be fragmented. Few references discuss a seamless integration of AI, KBE and CAD (an inevitable point in order to attain real design automation and iterative optimization).

Third, sustainability and environmental performance are the focus of most case studies, but only a few of them quantify environmental impact measures such as energy consumption, recyclability or life cycle assessment. This confines the "environmental" nature of nanomaterials to a concept rather than an assessable design factor.

From the application perspective, considered studies collectively suggest that AI and KBE can significantly facilitate discoveries and optimization of nanomaterials with predefined properties. But truly unlocking this potential in a quantitatively actionable way will require the development of standardized datasets, transparent sharing of models, and frameworks that contribute to bridging computational prediction with experimental validation. The integration of these factors would transform the nature of materials design from empirical-based to knowledge-based fashion with clear implications for cleaner production processes, circular materials economy or sustainable manufacturing.

C. Cross-domain Synthesis and Limitations

Through a cross-domain synthesis of the literature explored, some complementarities/ tensions can be identified between AI/KBE and environmental nanomaterial design. The AI-based methods are very successful in identifying complex coupling relationships between material properties and performance (especially when the data is abundant, e.g., adsorption model and photocatalytic optimization). However, these approaches usually lack interpretability and rely heavily on data quality, making them hardly reliable to be widely applied out of training configurations.

In particular, the KBE are focused on rule-based reasoning and design traceability and consistency such that they are particularly suitable for structural decision-making or CAD automation applications. They suffer from the cost of formalizing expertise and have low flexibility with fast developing material systems. From a nanomaterial point of view, most work concentrates on laboratory-scale validation under artificial conditions, and little is known about scalability or lifetime performance over realistic environmental variability.

The differing strengths and weaknesses described above indicate that neither AI nor KBE is complete in itself for the complex synthesis of environmental nanomaterials. If integrated into our lives, however, and balanced with real material constraints and a sustainable context, they become part of a balanced solution set that already includes the more robust tradition of design. This synthesis strengthens the need for hybrid architectures blending predictive intelligence, expert reasoning, and domain-specific validation.

D. Data-related Challenges: Bias and Domain Shift

Although data shortage is well recognized in the AI-based nanomaterial design, few literature has discussed the more profound challenges, i.e., dataset bias and domain shift. Dataset bias occurs when training data over-represent certain material classes, synthesis conditions, or performance ranges and results in models that are only accurate within limited design spaces. For instance, datasets can be skewed toward a particular type of experiment (e.g., lab-scale) or idealized conditions, which may bias predictions towards positive outcomes and ignore aspects such as decay, variability or failure scenarios.

Domain shift provides another challenge for the AI models trained under one experimental or simulation condition to be used in other environment, material composition and operational scales. In environmental nanotechnology, these shifts may be induced by varied contaminant concentration or pH/temperature, which may degrade model robustness seriously in the presence of real-life environmental variability.

Knowledge-based engineering (KBE) systems partly address these concerns by archiving expert rules and constraints; however, such systems are themselves restricted to the extent and conditions defined by the implemented knowledge. Solving dataset bias and domain shift requires complementary strategies that merge data augmentation, domain-aware learning, model incrementality with continuous updating and expert-guided validation. These challenges must be taken into account explicitly to translate AI–KBE approaches from laboratory conditions to the complexity of natural environments.

E. Transferability and Generalization Challenges

One of the primary impediments to the use of AI/KBE models for design within environmental nanomaterials is their lack of generality from one material class and set of environmental conditions to another. Typically, AI models are trained on narrowly defined datasets which relate to specific nanomaterials, routes of synthesis or operating conditions. Models developed for one material system such as metal oxide nanoparticles may not easily generalize to carbon-based or hybrid nanocomposites without retraining by use of substantial data augmentation.

The environmental dependence makes model transfer more difficult, as variables such as temperature, pH, composition of contamination and time of exposure can strongly change the behaviour of a material. Models trained in the lab have limited reliability when deployed into dynamic environmental conditions.

KBE frameworks are a partial solution to these limitations since they encode the know-how of experts, constraints and design heuristics that hold for any material class. Yet KBE systems are limited by the completeness and relevance of the knowledge base, and they need to be consistently updated as new material and circumstances proliferate. Such transferability challenges can only be tackled by hybrid AI–KBE techniques that integrate domain-informed learning with adaptive rule updating and iterative validation over a wide range of material systems and environmental conditions.

F. Interpretability and Explainability Challenges

Interpretability represents an essential need for the trustworthy implementation of AI-enabled models in environmental nanomaterial design. Although effective and efficient, a large portion of machine learning and deep learning models remain black boxes in the sense that they can generate accurate predictions with keywords but cannot describe how input parameters govern the responses of materials. In safety- or sustainability-critical use cases, for example in water treatment or pollution decontamination, lacking interpretability limits trust and scientific validation as well as regulatory acceptance.

The rule-based systems, on the other hand, have an explicit representation of rules as well as can trace the logic behind these decisions for that a group of experts are able to understand and verify the final design. However, KBE methods alone may oversimplify intricate material interactions which are better represented using data-driven AI approaches. The interpretability aspects of hybrid AI–KBE systems, therefore, become problematic especially when prediction as outputs are to be accompanied by explanations in terms of physical rationale or environment considerations.

Dealing with interpretability necessitates the combination of explainable AI (XAI) techniques, including feature importance analysis and rule extraction, with domain knowledge-driven verification methods. Improving explainability not only increases trust and usability, but also enables knowledge transfer between computational models and human engineers, which is crucial for the scalable and responsible deployment of intelligent nanomaterial design systems.

Explainable artificial intelligence (XAI) techniques have recently become an area of investigation to tackle the interpretability problems in material science applications. Such a feature-level attribution can be performed by using methods like SHapley Additive exPlanations (SHAP), which helps to understand the most important material descriptors or process parameters predicting the property. Attention type neural networks add interpretation where brighter parts mark significant interactions in complex material descriptors, whereas graph-based NN (GNN) explainers are especially promising for nanomaterials since they can capture atomic structure and inter-particle relations. While these XAI methods hold potential in enhancing transparency and trust, their implementation in the environmental nanometrial design is limited and isolated, highlighting a demand for widespread integration of explainability into AI–KBE workflows.

G. Future Research and Development Directions

Based on the knowledge gaps and challenges presented, we summarize prospects in this section for future study to push forward hybrid AI–KBE systems in environmental nanomaterial design.

1) Creation of Open, Curated Databases: Creation of open-access, large-scale repositories for environmental nanomaterials much like Materials Project or NanoHub is necessary. Such repositories should be created and populate with standardized descriptors, synthesis conditions, as well as performance metrics on how the sensor performs under various environmental conditions to train rigorous AI predictors.

2) Hybrid Intelligence Systems: Hybrid systems, which combine the best of human expertise (usually through KBE and/or expert system) with pattern recognition and scalability of AI, hold the future. These systems can enable interpretable, generalizable and context sensitive decision making in nanomaterial design.

3) Digital Twin and Real-Time Feedback Integration: Integration of AI-KBE workflows with Digital Twins virtual replicas of physical systems can provide real-time monitoring, predictive maintenance, and adaptive optimization to the field installed nanodevices (e.g., water treatment membranes, sensors). These models will be able to learn in real-time from sensor data, make updated design recommendations, and operate efficiently under volatile conditions.

4) Multi-Objective Optimization and Sustainability: Future AI-KBE platforms need to accept multi-objective optimization and should find a compromise between performance, cost, energy consumption, recyclability and toxicity. It is in line with the concept of circular economy, allowing the effective design and environmentally-friendly nanomaterials.

5) Alignment with Sustainable Development Goals (SDGs): There is a rare opportunity to integrate AI and environment-based nanotechnology research with global initiatives such as the UN Sustainable Development Goals (SDGs) notably SDG 6 (Clean Water), SDG 13 (Climate Action) and SDG 12 (Responsible Consumption & Production).

H. Challenges and Future Directions

Despite the great progress achieved in recent years with KBE applied to aerospace structural design, some under-investigated directions are expected to benefit both from a theoretical and practical viewpoint. Three important channels for future work will be:

1) Integration with Emerging Technologies: KBE combined with concepts like AI, ML and digital twin presents infinite possibilities. The integration of the predictive ML models as a part of KBE systems should also enable scaling the adaptive learning, by up-dating design rules and constraints as new samples are filled up. Also, the combination of KBE and digital twin can be used for in-time verification and online projectable optimization of structural performance all over not only design but whole product life cycle.

2) Standardization and Interoperability: However, even after advancement there is still a lack of standard for representing and exchanging knowledge. Work to be done in the future will develop an ontologydriven interoperable data model that bridges KBS platforms with CAD/CAE tools or enterprise PLM systems. Standardization would eliminate the need to push for duplicate development while making shared engineering across organizations and disciplines possible.

3) Addressing Knowledge Gaps and Uncertainty: KBE implementations today are mostly based on rule-of-thumb rules, that do not provide sufficient accuracy and result in an over-simplification of the stochastics in aerospace structures. Probabilistic and fuzzy logic extensions of KBE dealing with incomplete, confounding or changing knowledge may also be considered. This will improve the design automation and decision under uncertainity.

4) Sustainability-Oriented KBE Frameworks: Because of the importance of environmental issues in aerospace engineering, KBE systems shall address sustainability measures such as recyclability and energy consumption and life cycle analysis tools. The challenge would be how to build this information into more specific design rules, such that sustainability remains an emergent rather than a commanded need.

5) Human-Centric and Collaborative KBE Approaches: Hybrid systems that amalgamate automated reasoning and human expertise also holds potential. These could also apply to the design of collaborative KBE systems which increase the use of human-in-the-loop methods and automatically fuse efficiency with expertise. Such systems then can in turn be rendered transparent using explainable AI techniques and processes that provide explanations of trust-related reasoning.

6) Validation across Case and Industry Studies: Ultimately, further efforts are needed on the demonstration of KBE frameworks in an industrial context using large-scale validation techniques based around case-studies. The key will be to demonstrate cost, structural performance or design cycle time benefits that are universally applicable in the construction industry to move beyond academic prototypes.

To summarise, KBE research should go beyond technical development and consider the issues of interoperability, uncertainty management, sustainability and collaboration among human. By considering these dimensions, future research may place KBE as a fundamental of next-generation aerospace structure design.

I. Limitations of the Present Review

A few limitations need to be noted even though our attempt is made at an overall and systematic synthesis. One of the limitations to this review was that included peer-reviewed articles were conducted based on major scientific databases including Scopus, Science Direct, Web of Science, IEEE Xplore and Google Scholar. Therefore, studies presented in non-indexed journals or in patents, technical reports, industrial white papers may not be included.

Second, the review is based on described methods and results of published works and does not offer an independent experimental validation or benchmarking for AI–KBE frameworks. The result is that performances are extrapolated from the numbers given by the original authors.

Third, there may be a selection bias in focusing on recent and high-impact publications, which might underrepresent negative results or unsuccessful real-world applications that are less frequently reported. Lastly, as the artificial intelligence and nanotechnology landscapes continue to evolve rapidly, there may be new tools emerging or very recent publications without full representation at time of writing. These limitations should be taken into account when interpreting findings and conclusions of this review.

VII. CONCLUSION

The convergence of Artificial Intelligence (AI) and Knowledge-Based Engineering (KBE) presents a powerful paradigm shift in the design, development, and deployment of nanomaterials for environmental applications. As environmental challenges become increasingly complex and urgent ranging from water and air pollution to soil degradation and climate change there is a pressing need for smarter, faster, and more sustainable material innovation strategies.

This review has highlighted how AI techniques such as machine learning, deep learning, and generative modeling are enabling data-driven predictions of nanomaterial properties, optimizing design parameters, and guiding experimental efforts. In parallel, KBE systems are formalizing expert knowledge, automating routine design tasks, and ensuring consistency and regulatory compliance through rule-based logic. Together, these tools facilitate an intelligent design environment where environmental nanomaterials can be developed efficiently, reliably, and sustainably.

Despite significant progress, several challenges remain including data scarcity, lack of interpretability in AI models, software integration hurdles, and the need for holistic sustainability assessments. Addressing these limitations will require collaborative efforts across disciplines, including materials science, environmental engineering, data science, and computer-aided design.

Looking forward, the development of open databases, explainable AI, hybrid intelligence systems, and digital twins will accelerate the adoption of AI and KBE in environmental nanotechnology. Moreover, aligning these innovations with global sustainability goals will ensure that technological advancements also translate into social and environmental benefits.

In essence, the intelligent integration of AI and KBE into the environmental nanomaterial design lifecycle represents a critical step toward a cleaner, smarter, and more resilient future.

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