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Artificial intelligence and Expert Systems in Smart Materials: Current Trends and Future Frontiers

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ABSTRACT

Modern engineering and technology are increasingly being transformed by smart materials (ones that have intelligent responses and sensing capabilities to external stimulations). Recent developments in the field of artificial intelligence (AI) and knowledge-based expert systems (KBES) have greatly increased the process of discovering, creating, optimizing, and introducing such materials. This review will be a general overview of AI methodology and expert system in smart materials along with its present trends, enabling technology, and future prospects. The basics of the stimulus-response behavior, such as thermal, mechanical, electrical, magnetic, optical and chemical stimulation are initially addressed to develop scientific foundation of intelligent matter. The presence of AI-based methods (high-throughput screening, machine learning, generative adversarial networks (GANs), and physics-informed neural networks (PINNs)) is then discussed and it is shown that data-driven and physics-informed models become cheaper to experiment with but still achieve better prediction and allow the design of inverse materials. Simultaneously, the role of knowledge-based expert systems in the selection of materials, optimization, and the provision of assistance is examined, especially in the setting of Industry 4.0. Recent technological developments, such as computational materials science, real-time adaptive control, and digital twins are discussed in the light of the applications in smart textiles, energy systems, healthcare, and sustainable infrastructure. Lastly, new issues on data sparsity, multi-scale complexity, manufacturability, ethics and regulation are touched on, as well as a vision into the future of autonomous, self-healing, environmentally friendly smart material systems. This paper highlights the transformative power of AI and expert systems in bringing smart materials in laboratory applications to practical solutions and effects in the world.

1. Introduction

1.1 Foundations of Intelligent Matter: Definition of Smart Materials

Smart materials have been developed to react to external stimuli like temperature, pressure, light, humidity, and electric or magnetic fields. These materials have intelligent behavior since they alter their physical characteristics in real-time, and they can be utilized in diverse innovative applications in different industries. To give a few example, shape-memory alloys can be restructured to their initial shape upon heating following deformation, self-healing polymers will repair themselves autonomously and piezoelectric materials produce electricity when under mechanical strain.

Out of the contrast of the traditional material in which the material preserves its properties unless subjected to mechanical acts,

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smart materials are structured at the molecular or atomic scale to respond to the changes in the environment dynamically. Their versatility therefore boils down to this flexibility, which makes them suitable to advanced use.

Smart materials may have more than one functionality. One of the uses of thermochromic materials such as temperature indicators in devices and food containers is the color change caused by the temperature. Moreover, these materials may be self-controlling and changing under the impact of the environment. Examples include smart bandages that will be used to track the maintenance of the wound, and aircraft parts that will evolve their SCADA structure to suit changing environmental flight needs.

The necessity to realize sustainable products in addition to functional ones has driven the creation of smart materials, which can provide such solutions as the reusability of this material and its capacity to heal itself, minimizing waste. The industries that are being transformed by these materials include the healthcare sector, construction industry and even the automobile design, [1], [2] and [3].

An in-depth analysis of AI methods shows that, although machine learning is an excellent technology in terms of pattern recognition in large data sets, physics-informed algorithms such as PINNs provide more solid predictions when physical restrictions are taken into account. The result of this difference in abilities is the complementary nature of the uses of these methods in the study of materials science.

1.2. Historical Context and Development

The emergence of smart materials marks a significant advancement in materials science, driven by the Fourth Industrial Revolution (Industry 4.0). This era emphasizes materials that can actively respond to environmental changes, requiring adaptability, sustainability, and reliability. Research into intelligent materials began in the mid-20th century, focusing on materials that modify their behavior under specific conditions. The 1980s saw a rise in interest in piezoelectric materials, pivotal for sensor and actuator applications.

The fusion of artificial intelligence (AI) with material science has accelerated the discovery and optimization of smart materials, enabling machine-learning techniques for high-throughput testing and predictive modeling prior to laboratory experimentation. Large databases now support the correlation of extensive experimental data with theoretical concepts, facilitating the design of materials responsive to complex stimuli, including the use of generative adversarial networks (GANs) for customization.

However, commercialization of these materials faces challenges, requiring collaboration between scientists, engineers, and industry leaders to transition from research to practical applications. Despite these hurdles, smart materials are expected to play crucial roles in various sectors, such as healthcare and construction, by addressing evolving societal needs, [4], [5] and [6].

Although AI methods have allowed discovering smart materials much faster, there are still issues, including the sparsity of data and the high level of calculations required. The next steps in AI in materials science are to maximize these procedures to deal with these problems like combining machine learning with physics-based constraints.

1.3 Mechanisms of Stimuli-Response

The benefit of smart materials lies in the fact that they are able to modify and vary their characteristics when impacted by various external stimuli. This capability differentiates them with the old-fashioned materials and enables the possibilities of numerous applications. These materials can change their form, dimension or geometry, recoverably, or irrevocably, depending on the composition of the material and the kind of stimulus present, when subjected to a stimulus.

The smartest trigger perhaps used is temperature. An example is take shape-memory alloys (SMAs). These metals have the ability to spring back to a shape once it has been predetermined to do so when it is heated to a specific temperature. This is because changes take place in their crystalline structure, and this enables them to recollect the original shape. Similarly, shape-memory polymers (SMPs) are temperature responsive polymers which are used in medical devices as well as auto parts.

Light may also be a good stimulus. Specific materials which react to exposure to ultraviolet (UV) or near-infrared (NIR) light are known as changeable materials. Photoresponsive materials respond to light by modulating their properties and as such, it is possible to precisely control the behavior of these materials. A good example is photopolymers applied to 3D printing; they harden promptly when subjected to UV light making the production process simpler and allowing the creation of intricate shapes.

Another responsiveness is the chemical triggers. An example is the hydrogels that expand and contract when their surroundings change (e.g. change in pH or change in ionic concentration). Such a characteristic is invaluable in biomedicine, e.g., in drug delivery system where some strict release is reliant on conditions in the body.

Even finer control is offered on smart materials by means of electric and magnetic stimuli. In piezoelectric materials, electric charges are produced when under the action of mechanical forces, and this can be used in sensors and actuators in many industries. Equally, the magnetic field-sensitive materials can be used to modify the physical condition of its materials, which have the potential to be applied in targeted delivery of drugs and other medical-related issues.

This amazing variety of responsiveness does not only enhance the usefulness of smart materials, it also assists in saving energy since it is possible to accurately control the way the material reacts. The opportunities of the groundbreaking innovations continue to increase as scientists are exposed to new material blends and fresh stimuli, [1], [6] and [7].

The combination of AI and quantum computing can also discover new material with uncharted qualities, including the type needed in the coming-of-age energy storage technologies. Moreover, optimization of the material lifecycle management made possible with the help of AI can add to more sustainable manufacturing.

Finally, AI and smart materials convergence show promise of revolutionizing industries because it can provide autonomous, adaptive systems of materials. By overcoming the existing constraints and emphasizing on interdisciplinary partnerships, the advancements in smart materials in the future would pave the way to the new sustainability and efficiency achievements in such spheres as healthcare, construction, and energy.

2. AI Methodologies in Material Discovery

2.1 High-Throughput Screening Techniques

Materials discovery has undergone major changes in time due to the application of high-throughput screening (HTS), which allows fast investigations of a large number of materials. Historically, the development of the new materials was done through lengthy and costly experiments, yet the development of computational methods, especially the computational throughput (HTC), is is now reducing the challenges. In order to attract investment, HTC improves large-scale simulations with automation and scaling of simulations, which consequently provides researchers with an opportunity to perform first-principles calculation of large chemical and structural families. The main benefit of HTS is that it can provide large amounts of data due to the simultaneous implementation of experiments and therefore speed up the discovery of materials with favorable characteristics. At the core of this process are first-principles schemes, such as the density functional theory (DFT) as they can offer predictable information on the electronic organization, stability and reactivity that is not dependent on experiment. Consistently made changes in composition and structure result in extensive data bases that scientists can tap to retrieve materials that can be used to meet a particular need.

This is further improved by integrating the machine learning with the HTC, thus being able to make predictions about the characteristics of a previously untested material. Older methods like clustering and inverse design assist in determining the electronic properties and unearthing the patterns in large volumes of data, whereas generative models with the assistance of the inverse design help to create new compositions according to the performance requirements. Another notable use of HTS is in energy storage, especially in lithium-ion batteries, where a fast screening enables scientists to test electrode materials in respect of voltage, stability and capacity quickly, resulting in the discovery of improved compounds. HTS. also treats complex systems such as high-entropy alloys, in which the number of possibilities of combinations may exponentially grow. This is supported by the effectiveness of HTS through the presence of strong computational environments that support automated generation of structures and analysis of property and data, which supports consistency in large-scale simulation problems. Detection of new materials becomes not only possible, but efficient with the help of special platforms making screening of vast of them possible. In general, HTS enhances innovation through reducing uncertainty and speeding up data-based approach and automation of materials science, [8].

2.2 Generative Adversarial Networks (GANs) in Material Design

Generative Adversarial Networks (GANs) have been the new revolution in materials design which mainly concerns smart materials. These networks are two rival models an adversary and a discriminator which collaborate with one another. The samples of new data are made by the generator and the authenticity of the new data samples is evaluated by the discriminator through the comparison to the actual data. This back and forth forces the generator to develop and become better with time and deliver better outputs.

GANs present an opportunity to traverse enormous chemical surfaces in a highly efficient manner. They have the ability to come up with new material to satisfy certain property demands by not necessarily referring to the available datasets. Indicatively, GANs have the potential to produce hypothetic compounds that fit the ideal scenario of structural/functional specifications, which is invaluable in producing productions of materials applicable in soft robots or biomedical equipment. GANs can identify structures that can provide greater mechanical strength or biocompatibility by emulating complicated interactions and behaviors.

The recent breakthroughs demonstrate that GANs have the potential to fill the gaps existing in the experimental data due to its lack of the latter. This accelerates a discovery and enhances our understanding of the relationship of structure with performance. On the one hand, the GAN-related AI-aided designs resulted in shape-memory polymers with increased tensile strength and self-healing abilities, which was an unmistakable improvement in a number of performance indicators.

The integration of physics-based constraints in GAN goes a notch higher in enhancing its reliability. The step makes the materials produced conform to the laws of physics and this helps to minimize the possibility of making unrealistic or impossible candidates. It is also used in illuminating the impact of specific structures on the property of the material and consequently, results are more interpretable.

GANs are also exceptionally bright in the approach of inverse design, in which they effectively sample vast chemical spaces to discover new inorganic materials. They may utilize such networks to generate valid and novel chemical candidates at sizable rates when conditioned upon large crystal databases. Automation of this process reduces the time and cost as opposed to the conventional technique of experimentation.

Integrating GANs with other machine learning, such as variation auto encoders (VAEs) is associated with added advantages. Such integration enables scientists to design richer material maps which can be fine-tuned to the desired characteristics, i.e. the conductor achieves a hairy response to multiple individual design criteria. The resultant output is the multiple axis polish toolkit.

Overall, it can be concluded that Generative Adversarial Networks provide new avenues in accelerating materials design. Using deep learning, they allow them to develop custom solutions that are fine-tuned to the requirements of the smart materials science, [9], [10], [11] and [12].

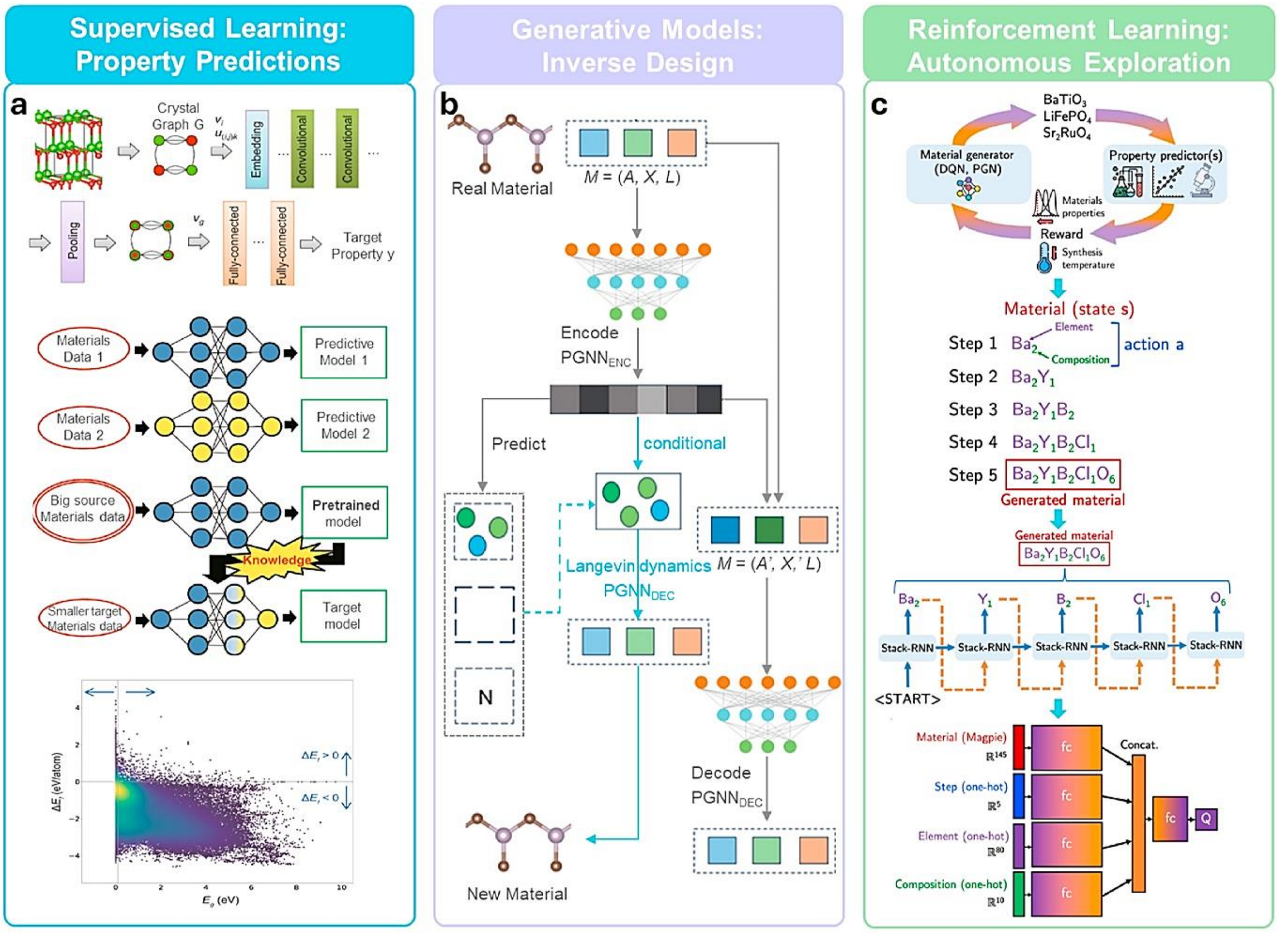

Figure 1. Main Methods and Paradigms. (a) CGCNN-based transfer learning beats the challenge of data scarcity in supervised learning predicting material properties, (b) Generative modeling invents inverse design and discovery of novel 2D Materials, (c) Deep reinforcement learning beats the challenge of discovering novel inverse inorganic materials, [10].

2.3 Physics-Informed Neural Networks

Physics-informed neural networks (PINNs) are neural networks that combine classical physics and andragogy into an unprecedented innovation in changing materials science. Such networks have inbuilt physical equations inside them and predictions include established physical laws. This method works particularly well on smart materials, where the relationship between material behaviors and other underlying physical phenomena are complex and capture the complexity of the correlation.

The use of physics in training makes PINNs more accurate and interpretable at the same time. In contrast to the conventional machine learning models that need huge data sets and may not be able to generalize, PINNs rely on physics expertise to inform learning. This would come in handy especially when there is no sufficient data, therefore, these networks would be able to work even in unfamiliar circumstances.

PINNs are highly effective in the case of inverse design, during which researchers desire the answers to a question mix of microstructural features into the preferred properties on a bulk scale. By framing it as a constrained optimization, researchers have the option to combine data information with physical laws to find the best possible solutions, and it takes shorter and more reliable in search of the best solution than the traditional approach.

In addition to predictions, PINNs assist in real-time practical and control of smart materials working. Sensors with feedback can be discussed as the materials with sensor feedback that can be adjusted in the form of PINNs over the changes in temperature or pressure. This has the benefit of allowing materials to dynamically adjust their performance in response to changing conditions or in response to the needs of the user.

Greater supercomputing capabilities have increased the scope of use of PINNs, which are used in structural health monitoring and in durability risk assessment. Physics-informed techniques with graph modeling are perfect to acquire complex structure-property relationships that are essential to next generation materials.

PINNs can also be used together with artificial intelligence methods such as reinforcement learning. With this combination, it is possible to optimize the closed loop so that synthesis processes get better with improved experiments and predictions in physics. Consequently, scientists discover a larger compositional space more effectively whilst being constrained by physical laws.

Scaling PINNs to larger and more complex systems, as well as training it with reduced cost, are still difficult. Incidents of algorithmic improvements and the ability to measure uncertainty ensure further improvement in their credibility and applicability. Finally, PINNs combine both models based on data and models based on fundamental physics, and Waveguide these in the design and optimization of materials that are both interpretable and physical, [2], [8] and [10].

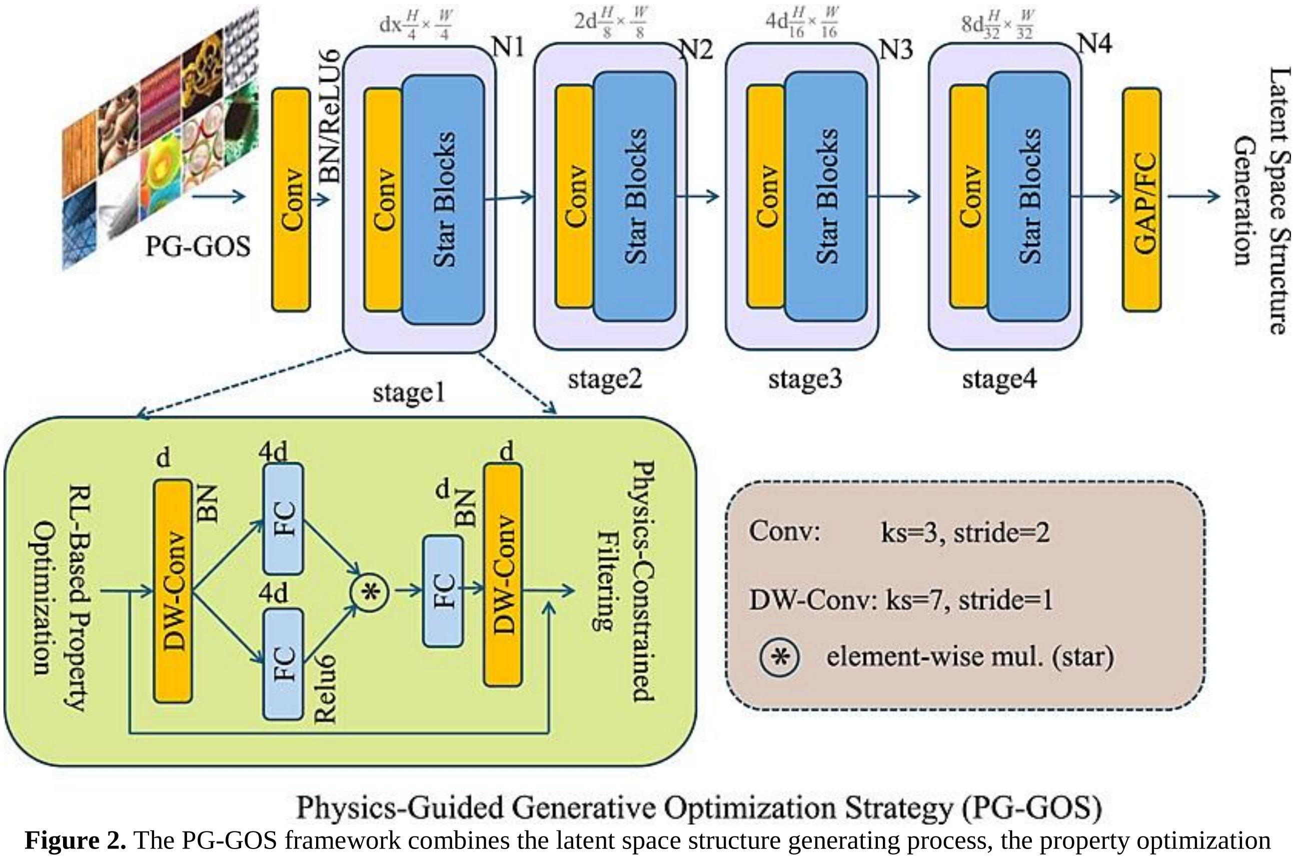

Figure 2. The PG-GOS framework combines the latent space structure generating process, the property optimization process, which is conducted by reinforcement learning, and the filtering procedure, which is held by the physics constraint. All these constitute a whole pipeline of inverse material design. Given a latent initial vector, a generative model predicts candidate structures that are optimized through reinforcement learning having been mapped to the latent

initial vector all to satisfy target properties balancing structural stability. Designs that are physically invalid are filtered using physics-based constraints and thus, the materials that are generated are both high-performing and physically plausible. It is an excellent strategy that allows probing into new materials in an efficient and reliable manner, [8].

Table 1: A comparative study on our approach and the SOTA methods on 2DMatPedia and Jarvis-DFT datasets, [8]

Model	2DMatPedia dataset			JARVIS-DFT dataset		
	MAE (eV) ↓	**RMSE (eV) ↓**	**R^2 ↑**	**MAE (eV) ↓**	**RMSE (eV) ↓**	**R^2 ↑**
CGCNN	0.342	0.511	0.78	0.364	0.532	0.75
SchNet	0.319	0.484	0.81	0.335	0.505	0.79
Transformer	0.298	0.451	0.83	0.312	0.470	0.81
Ours	0.251	0.392	0.87	0.267	0.418	0.85

Table 2 compare different AI methods (including High-Throughput Screening, Generative Adversarial Networks, and Physics-Informed Neural Networks) assuming the main aspects, including applicability, accuracy, cost of computation, limitation, and strengths.

Table 2: Comparative analysis table: AI techniques for smart materials

AI Methodology	**Description**	**Applicability**	**Strengths**	**Limitations**	Computational Cost	Data Requirements	**Example Applications**
High-Throughput Screening (HTS)	A method for rapidly testing and evaluating large numbers of materials for desired properties.	Primarily used for material discovery, especially in polymers and alloys.	- Quick screening of vast material libraries. - Cost-effective for initial stages of material discovery.	- Limited to pre-existing material databases. - Does not account for complex interactions in real-world environments.	Low to moderate, depending on the number of materials and tests involved.	Requires large, high-quality datasets of material properties.	Screening of candidate materials for battery electrodes, catalysts, and composites.
Generative Adversarial Networks (GANs)	AI model that generates new material designs by learning from existing datasets.	Useful in generating novel material structures, particularly in complex systems.	- Can generate novel materials that have not been discovered before. - Capable of learning from large datasets.	- Needs large and diverse datasets to perform well. - Difficulty in generating physically realistic designs.	High, as GANs involve complex neural network architectures.	Requires large datasets with high-quality and diverse material property data.	Generating novel polymers, composites, and biomaterials for specific applications.
Physics-Informed Neural Networks (PINNs)	AI model that integrates physical laws (e.g., thermodynamics, elasticity) into the learning process.	Ideal for materials with known physical behaviors and laws.	- Integrates physical laws into the model for better accuracy. - Can model	- Computationally expensive for large systems. - May struggle with complex, nonlinear material systems	High, particularly for solving differential equations and large systems.	Requires high-quality data that adheres to physical laws or synthetic data to train the models.	Modeling the mechanical and thermal properties of materials, predicting material behavior

AI Methodology	**Description**	**Applicability**	**Strengths**	**Limitations**	Computational Cost	Data Requirements	**Example Applications**
			complex material behaviors more effectively than traditional ML methods.	that do not fit well with predefined physical laws.			under stress.

HTS can do best with materials at the initial stages of development and does not always do well with complex interactions when applied in practice.

The positive thing about GANs is that they are capable of creating new materials, but they require vast, vast datasets and do not reliably create competent designs.

PINNs embed known physical laws into AI architectures, which yields high accuracy to systems that are driven by physical laws. However, they are also computationally costly and might experience difficulties in nonlinear and complex cases.

3. Knowledge-Based Expert Systems (KBES) in Selection & Design

3.1 Framework and Architecture of KBES

The Knowledge-Based Expert Systems (KBES) is critical in materials science and engineering. They systematize the knowledge with specific specialization to enhance decision making. The knowledge base is the key feature of a KBES and it holds the domain-specific information, best practices as well as expert rules. This structured warehouse can be used to locate applicable data with ease that is useful in making effective decisions.

The KBES would generally entail the body of knowledge, an inference engine, user interface and a description module. The knowledge base holds elaborate information concerning the material property, stimulus response and interaction, as well as heuristic rules to make decisions. Physics-inspired models, such as Physics-Informed Neural Networks, can contribute to the increased accuracy of the predictions and make the results more consistent with the fundamental principles.

The inference engine utilizes logical rules on the knowledge base in order to draw new conclusions or action suggestions. It can either be forward-chaining, beginning with known facts, or can be backward-chaining, starting with a goal and trying to disprove it. These forms of reasoning imitate the thinking of the experts, and they enhance the ability to solve the problems.

The interface plays a vital role in the interaction of the user. It gives users the chance to interact with the system in a natural way, and visualize information with complex representations, thus increasing real-time understanding. The presence of the explanation module inspires transparency as the explanation behind the decisions is seen, leading to the trust of the user, particularly when making serious decisions.

The ability to conduct rapid analysis of large material libraries based on the rules created by experts allows KBES to accelerate the process of material selection and eliminate the needless trial and error, which lead to high expenses. The knowledge base and inference rules are regularly updated to ensure that the system is in line with new scientific findings and technology advances, which is necessary in the contemporary industrial environment such as Industry 4.0.

Also, the use of KBES in combination with machine learning helps systems to acquire new knowledge and modify rules as time progresses. This is an efficient, sustainable design of materials, which is constantly enhanced by this hybrid technique and ensures compliance with modern needs, [2], [6], and [15].

3.2 Applications in Material Selection and Optimization

Knowledge- Based Expert Systems (KBES) are also important in the process of selecting and optimization of smart materials. They follow a system of structure that comprises of a knowledge base, inference engine, user interface and an explanation module. The knowledge base brings together the specialized information concerning the properties and uses of materials. Complex problems can be solved using forward and backward chaining, logical methods of reasoning.

KBES analyze materials in practice through comparison between physical and chemical characteristics and pre-established standards. To illustrate, in designing smart textiles using nanomaterials, the systems direct engineers to make decisions with the appropriate mechanical strength, flexibility and environmental conferralence. A decision makes it easier to embed expert knowledge which may provide practical suggestions.

KBES also make great choices of material to be used in energy storage specifically the battery of advanced type wherein charge capacity and cycle life are of utmost importance. The use of artificial intelligence together with high-throughput screening enhances candidate analysis and makes better decisions. In addition, machine learning enables such systems to enhance evolvingly as they are learning based on previous decisions and fresh data. Reinforcement learning becomes more precise on the recommendations made in the results of experiment.

Other than energy, KBES can be used in structural engineering and biomedicine, where health and mechanical requirements have to be fulfilled. Expert systems are used to examine massive databases in order to make sure that materials are of good quality and conform to the regulations. They are also involved in coming up with new smart materials formulations, optimizing the formulations prior to physical testing. As an example, they determine the most ideal composites on shape-memory polymers of medical equipment’s or adjustable furniture surfaces.

Knowledge AI technologies are combined with real-time adaptive control technologies to manipulate manufacturing or use in real-time to maximize efficiency and reliability. All in all, KBES optimize the choice of materials and innovation in areas of smart and supportive materials, and supplement designers and engineers with state-of-the-art decided support tools, [6], [10], and [16].

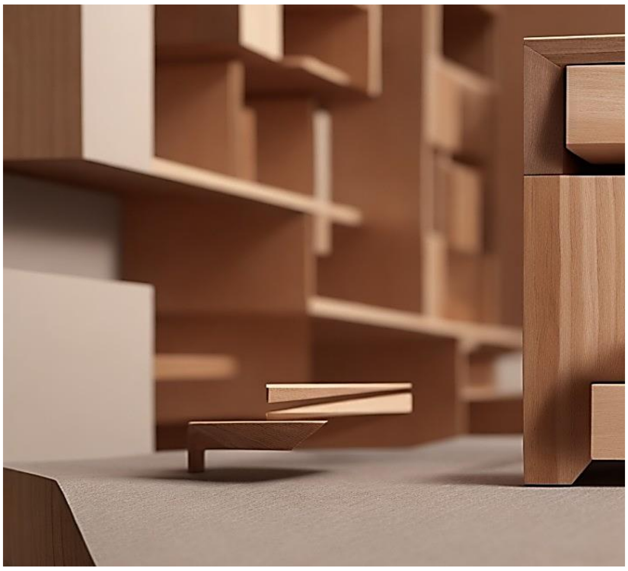

Figure 3. AI and Smart Materials: A Winning Combination in Furniture Development, [1].

4. Current Technological Trends

4.1 Advances in Computational Materials Science

The new trends in the science of computation have dramatically changed the procedure of designing, optimizing and applications of materials in different disciplines. One of the most important developments is high-throughput computing (HTC), which allows researchers to establish all the materials that are relevant in large data sets efficiently. This enhances the discovery of materials in a shorter time and enhances to a greater degree the predictive models so that it is easy to identify new materials that have a particular desired property with the aid of data-driven methods. The conventional experimentation is usually hindered by the cost and time, which can be solved using computational approaches.

The development of generation frameworks of digitized material designs makes researchers more predictive, uniting machine learning with the computational technique to reduce the guesswork and lower the number of trials and errors. The key figure of this novel landscape is the Materials Genome Engineering (MGE) that combines new models of experimentation with sophisticated computing to accelerate the material design. It centers on multi scale modelling, automated lab procedures as well as efficient data management systems as a way of fostering effective development procedures.

The leading force of these developments is artificial intelligence (AI), according to which AI algorithms can study a large body of data and discover transient patterns and trends. Generative AI, such as, allows the researchers to produce very new materials in accordance with the data they have as opposed to just making changes to the known materials, something that has considerable implications to the likes of personalized medicine.

The current advancement in this industry is encouraged by the innovative projects, including digital twins, which are virtual counterparts of physical systems, and which are permitted to track modification of materials in their lifecycles, in real-time. The interrelations between universities and industries also promote the innovation by establishing standards to follow in terms of sharing information and increasing the compatibility of research tools.

In general, these innovations indicate a stepwise-interrelated approach in material creation wherein human innovativeness is supplemented by computer capabilities. The combination of machine learning technologies and big data analytics may open the door to the innovations of smart materials that can be used in healthcare and energy, manufacturing, etc., [8], [9] and [15].

4.2 Real-Time Adaptive Control Technologies

The real-time adaptive control technologies represent a huge improvement in the interaction of smart materials with the environment. Following artificial intelligence (AI), such systems modify their characteristics or behaviors in real time, based on real-time streams of data to enhance performance, as well as expand their application possibilities.

One of these vivid examples is smart clothes. Smart technology that relies on AI detects temperature, pressure, and moisture levels amid their occurrence by integrating sensors into the device board. This information is then processed by the AI and the fabric is able to change its thermal insulation or moisture-wicking capabilities within seconds. This live feedback makes comfort and functionality available depending on the situation of the wearer.

Complex hybrid learning approaches slightly increase the sophistication by forecasting intent by continual analysis of body-fabric interaction. Carbon-based fibers with neural networks are able to alter their conductivity or resistance dynamically, without being directed to do so. As an example, they could feel a person doing something or taking a break and adjust thermal features to that end, which is also the beginning of the new autonomous adaptive design.

Adaptive control is converting energy systems that are in form of smart materials besides clothing. This is based on machine learning, which smart photovoltaic (PV) units use to track the sun in the most effective way, and control the flow of power. These are the systems that can program the panels continually to adapt to variations in the weather or shadows so that the maximum energy would be collected over the day. Reinforcement learning allows such systems to learn through the environment and improve their performance with time.

Blockchain also cooperation with AI enhances the decentralized energy grids. This is a collaboration that helps to ensure the transparent trading of excess energy which is yielded by smart PV systems. In the meantime, it ensures both the energy production and storage become intelligent on the dynamism of real-time data to ensure that the operations become more reliable.

These technologies are also accelerated by the development of computers. One example is quantum computing, which promises to solve complex material behavior that is too difficult to solve using the classical methods. The fact that it can work with massive amounts of data at a quicker rate, facilitates faster and more efficient decision-making that is required in real-time adaptation.

The merging of AI-based analytics and the control system is transforming sectors such as healthcare, energy and consumer goods. They form intelligent spaces that, together, do not simply react but predict the needs of the users and establish the new level of interactivity in technology, [9], [10], [15] and [16].

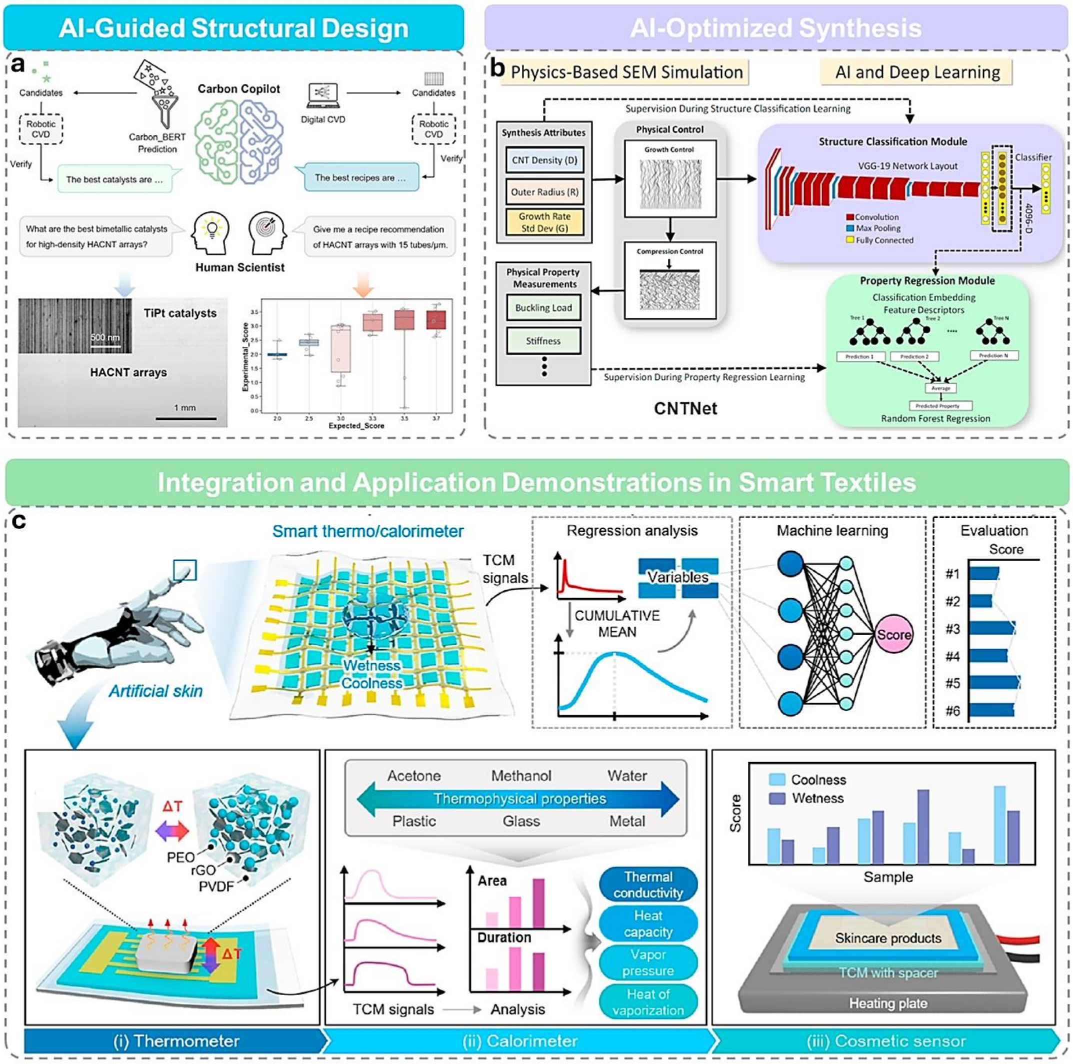

Figure 4. Smart Textiles with AI-controlled Carbon-based Nanomaterials. AI-controlled CARCO platform to structural design and property functionalization of carbon materials, (a), AI-optimized CNT Net platform to image-guided classification and property prediction in CNT forest synthesis, (b), Schematic of intelligent health monitoring system of multifunctional textile sensing, [10].

5. Future Frontiers and Theoretical Limits

5.1 Emerging Challenges in Smart Materials Integration with AI

The introduction of AI into smart materials creates an arsenal of challenges that should be overcome to create smooth and practical usage. A significant challenge is related to data. Material science AI models can work best using large and clean datasets, whereas a large amount of data or noise frequently affects small datasets because of the intricate nature of material design and testing. Such deficiency may happen as a result of overfitting or falsification of material characteristics by AI. That is why it becomes necessary to develop AI techniques which can work with incomplete/imperfect information that is highly reliable.

Smart materials also demonstrate a shift behavior with a vast difference in scale, that is between atomic to visible propagation. This is a multi-scale complex that makes it difficult to forecast their performance in various situations. The predictions provided by using some sophisticated models, such as the Physics-Informed Neural Networks (PINNs), will have a chance of being more accurate and obey the laws of nature. Nevertheless, the methods require further adjustments and experiments to make them work properly in all scales.

Problems get complicated during the production stage. The synthesis or the recycling of the material may introduce unwanted elements that will muddle the consistency of the material. This requires strict oversight in the manufacturing sector and the ability to monitor in real-time which AI can do, but only when its application can overcome the existing challenges.

There are additional challenges of integrating different AI systems per se. Because various AI tools are typically associated with distinct frameworks and assumptions, it is challenging to integrate them into the existing material working streams. The effectiveness of the entire system can be questioned in the absence of a smooth compatibility.

Correctness and morality are also questions of concern. As intelligent materials become independent in the context of evolving around the surrounding environment, there should be a set of clear rules on how they will be used in various industries. It is the problem of safety versus innovation, i.e., the collaboration between lawmakers, scientists, and leaders in the industry should be the key.

Trust-worthiness by the users is also a factor. Individuals can be reluctant to adopt smart materials in accessible products such as medical equipment or technology fearing the security or reliability. Development of confidence requires the availability of truth and good evidence of reliability.

Lastly, teamwork is the key in conquering such obstacles. Academic-industrial partnerships promote the sharing of knowledge and lead to the appearance of new ideas. The share of knowing how to work with computers, design, and user experience helps to develop combined strategies that stakeholders may use to drive smart materials forward along with AI progress, [2], [9], [10], [11] and [17].

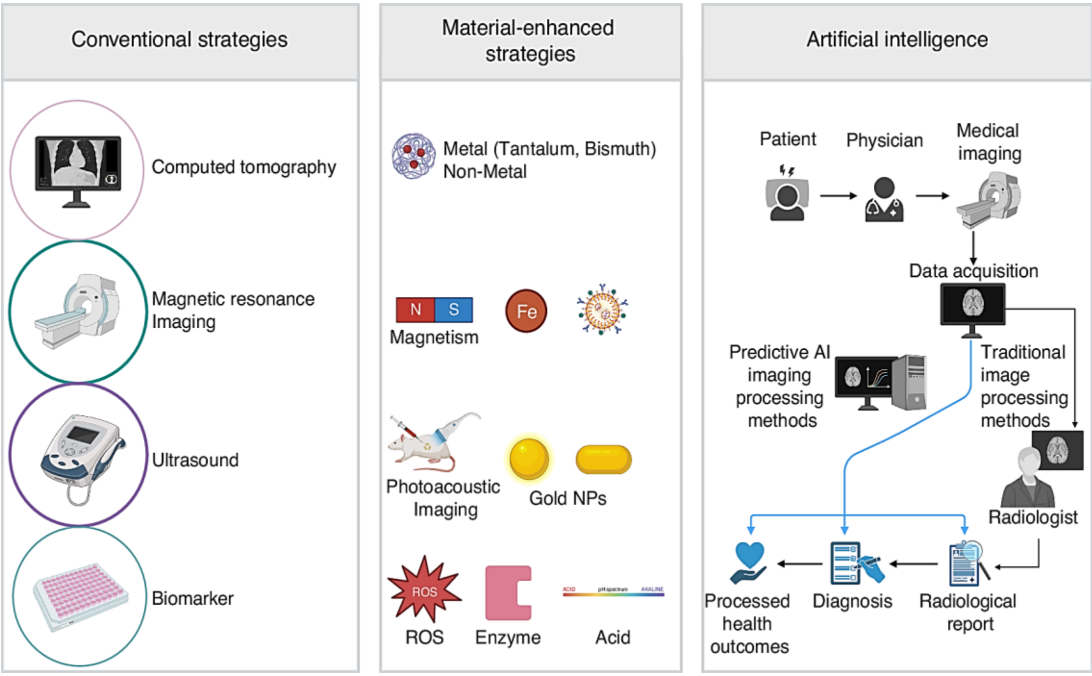

Figure 5. Diagnostic proposal of the traditional, material-enhanced, and AI-enforced solutions concerning OA diagnosis, [9].

5.2 Potential Impacts on Industry and Society

The use of artificial intelligence (AI) coupled with smart materials will transform different industries and social organizations. Among the prominent benefits is the increased speed and efficiency of the manufacturing processes that become possible due to the materials science computations that allow exploring the vast number of materials in a very brief period of time. This development contributes to the reduction of errors and precision and enables companies to create complicated parts faster and more cost-efficiently with the help of automation created by AI.

In construction, automotive, aerospace, electronics and other fields, the adaptive materials which react to the environment in real-time exhibit better wear in cases of extreme weather conditions. Technologies such as self-healing materials, besides lowering the cost of maintenance and increasing the lifespan of the infrastructure, also demand less human intervention. It is said that AI-controlled materials are finding use in the architectural design and urban planning of buildings to facilitate fewer energy and resource consumption that favors sustainability. It has been found out that these technologies may result in the saving of energy of between 18 to 35 percent and a roll of perceptions of carbon emissions during the life cycle of a building that will boost corporate perceptions of social concerns.

Reimbursement is also conspicuous because AI in conjunction with smart materials enhances efficiency and lessens overheads. This synergy makes product launch and innovation quicker and data analytics makes things more responsive on the market. As a result, there is a new demand on data science and materials engineering projects emerging and provision of changes in the educational curricula to match the changing demands of the work force is necessary. Moreover, intelligence materials that operate on AI can enable the city planners, engineers, and experts to collaborate on the issues pertaining to climate-resistance in the global context, with the goal of developing solutions that would be functional and environmental, at the same time.

Nevertheless, the developments raise regulatory issues especially- on product safety and access to the advantages in a fair manner. The key to the successful implementation of AI and smart materials is based on responsible and inclusive practices, which will mark a new epoch in production, building, and sustainability, [3], [4] and [19].

5.3 Vision for Next-Generation Smart Materials Systems

Since industries are moving ahead to achieve improved efficiency and sustainability, the future of smart materials is in the combination of sophisticated materials science and artificial intelligence. This combination will attempt to transform materials into active partners as opposed to passive elements in any given complex systems. The task is to design materials capable of self-adjustment and optimization of their operation based on real-time data and facilitate the environmentally friendly interest.

In the future, AI will be used to spearhead significant advancement in smart material design. Predictive models will also allow the scientists to predict the behavior of materials under various conditions and this will mean that one can design properties that are unique to certain applications. This information-based approach will accelerate the process of discovery and minimize waste and enhance performance.

The self-healing material can be real in the near future because the AI can replicate the biological process of healing. These materials would feel any type of damage and repair themselves without any external assistance, increasing their life and reducing the maintenance cost. This sort of breakthrough is fitting well in the ideals of the circular economy; aimed at resource saving, and the promotion of sustainability.

The smart material performance in the changing environments will be based on real-time adaptation. Using the artificial intelligence adjustments and constant sensing, smart buildings or wearable devices might change their functioning according to the needs of the users or regarding the changes of the environment. This will significantly enhance ease of the users and decreasing energy consumption in various industries.

As increasing focus on green innovation is placed, future smart materials will incorporate sustainability into them. Renewable and bio-derived components should be used with conventional production to produce products that would offer the best performance, which were environmentally friendly. The ability of AI to analyze the environmental data enables smarter decisions in the approach of material design to end-of-life processing.

Once these technologies are mature enough, collaboration within industries, among academia, and the government will bring new sophistication. Connected car systems will be used from healthcare monitors to self-driving cars as smart material systems are interconnected. Teamwork will also play a major role in overcoming regulatory challenges in the implementation of advanced technology.

On the whole, the perspectives of the next-generation smart material systems are comprehensive. It is not only that AI will enhance material qualities but also assist in achieving the sustainability goals. A focus on flexibility, independence, and sustainability will guide us to the future of smart solutions that fit multidimensional challenges in the society, [10], [13], [17], [18] and [19].

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