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Artificial Intelligence–Driven Frameworks for Accelerated Materials Discovery in Energy and Sustainability Applications

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Abstract: The discovery and optimization of advanced materials for energy and sustainability applications have traditionally relied on time-intensive experimental and computational workflows. Recent advances in artificial intelligence (AI), particularly machine learning and data-driven modeling, have enabled a paradigm shift toward accelerated materials discovery. This paper presents a comprehensive AI-driven framework designed to streamline the identification, prediction, and optimization of functional materials for energy storage, conversion, and sustainable infrastructure applications. The proposed framework integrates materials databases, feature engineering, supervised and unsupervised learning algorithms, and iterative validation loops to reduce experimental cost and discovery time. Case-oriented analyses illustrate how AI models can predict key material properties such as bandgap, thermal stability, catalytic activity, and mechanical performance with high accuracy. Furthermore, the study highlights the role of explainable AI in enhancing model transparency and guiding experimental decision-making. Challenges related to data scarcity, model generalization, and integration with laboratory workflows are critically discussed. The findings demonstrate that AI-driven materials discovery not only accelerates innovation cycles but also supports sustainable development goals by enabling the rapid deployment of eco-friendly and high-performance materials. This research contributes a scalable and adaptable framework suitable for next-generation energy and sustainability-oriented materials research.

Keywords: Artificial Intelligence, Materials Discovery, Sustainable Materials, Energy Applications, Machine Learning

1. Introduction

The global demand for sustainable energy systems and environmentally responsible technologies has intensified the need for rapid discovery of advanced functional materials. Materials underpin nearly every technological advancement in renewable energy, energy storage, carbon capture, and sustainable construction. However, conventional trial-and-error experimentation and first-principles simulations are often limited by high costs, long development cycles, and restricted exploration of the vast chemical design space [1]. Artificial intelligence (AI) has emerged as a transformative tool capable of overcoming these limitations by enabling predictive modeling, pattern recognition, and optimization across large and complex datasets. The integration of AI into materials science has given rise to the field of materials informatics, which leverages data-driven approaches to accelerate materials discovery and deployment [2]. This paper proposes an AI-driven framework tailored for energy and sustainability applications, emphasizing scalability, interpretability, and real-world applicability. Unlike isolated algorithmic studies, this work presents a holistic pipeline that connects data acquisition, learning models, and experimental feedback. The objective is to demonstrate how AI can systematically reduce development timelines while improving material performance and sustainability outcomes.

2. Background and Related Work

Early applications of machine learning in materials science focused on property prediction using handcrafted descriptors and regression models [3]. With the growth of open materials databases such as the Materials Project and Open Quantum Materials Database, more sophisticated deep learning approaches have been introduced [4]. Recent studies have applied convolutional neural networks to crystal structure representation, while graph-based models have shown promise in capturing atomic-level interactions [5]. In energy applications, AI has been successfully employed to discover high-capacity battery electrodes, efficient photovoltaic materials, and robust catalysts for hydrogen evolution reactions [6]. Despite these advancements, many existing approaches remain domain-specific and lack integration into a unified discovery framework. Furthermore, issues related to data bias, model explainability, and experimental validation continue to hinder broader adoption [7]. This study addresses these gaps by proposing an end-to-end AI-driven framework emphasizing sustainability-focused materials research.

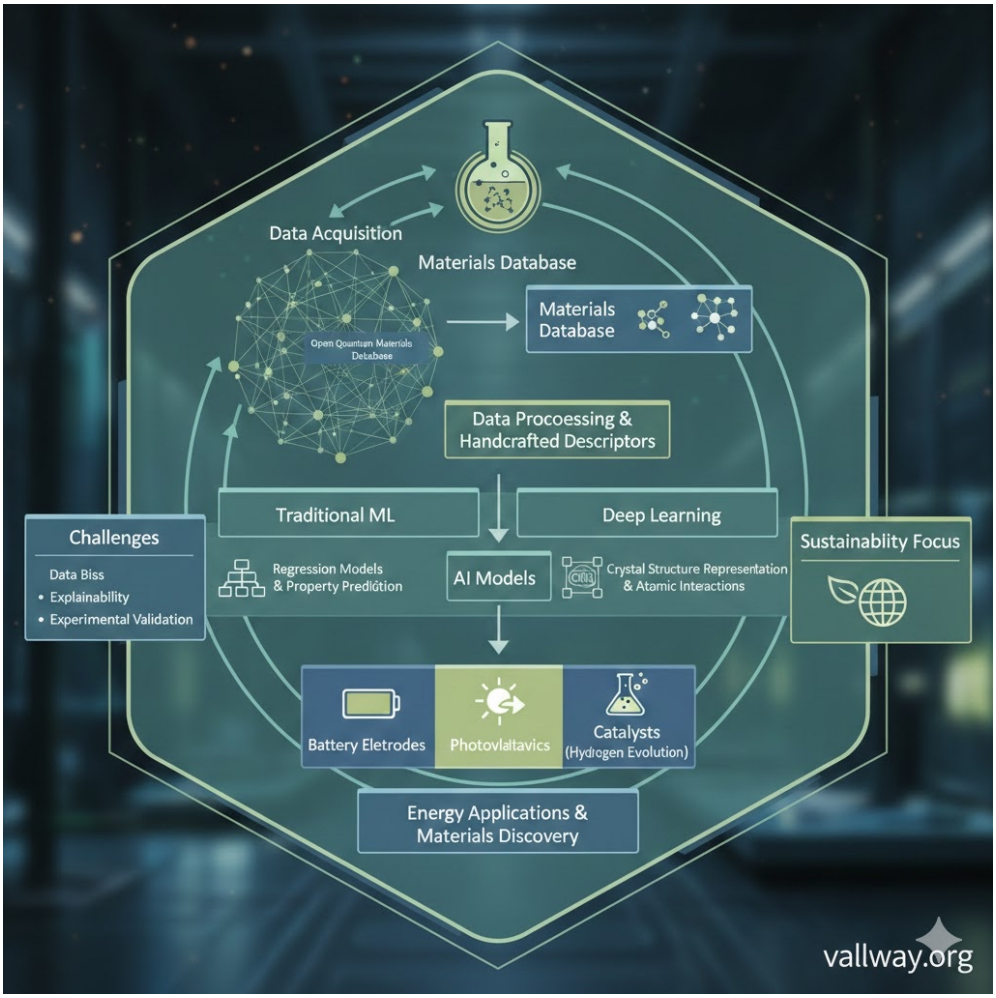

Fig. 1 Energy applications and material discovery

3. Proposed AI-Driven Materials Discovery Framework

The proposed framework consists of five interconnected layers: data acquisition, feature representation, model development, validation, and deployment.

Data Acquisition and Curation

High-quality data is the foundation of effective AI models. Experimental datasets, computational simulations, and literature-mined data are integrated into a centralized repository. Data preprocessing techniques such as normalization, outlier removal, and imbalance correction are applied to enhance reliability [8].

Feature Engineering and Representation

Material features include compositional descriptors, structural parameters, thermodynamic properties, and processing conditions. Advanced representation techniques such as graph embeddings and learned descriptors are employed to capture complex material relationships [9].

Machine Learning Model Development

Supervised learning models are used for property prediction, while unsupervised learning aids in materials clustering and design space exploration. Ensemble learning and deep neural networks improve prediction robustness across diverse material classes [10].

Validation and Feedback Loop

Model predictions are validated through cross-validation and selective experimental verification. Feedback from experiments is reintegrated into the dataset, enabling continuous model refinement and active learning [11].

Deployment for Sustainable Applications

The framework supports deployment in real-world research environments, enabling rapid screening of candidate materials for batteries, solar cells, catalysts, and sustainable construction materials.

4. Applications in Energy and Sustainability

AI-driven discovery has demonstrated substantial impact across multiple sustainability domains. In battery technology, AI models have identified novel electrode materials with enhanced energy density and stability [12]. In photovoltaics, AI-assisted screening has accelerated the discovery of perovskite compositions with improved efficiency and reduced toxicity [13]. Catalysis for carbon capture and hydrogen production has also benefited from AI-guided optimization, reducing reliance on rare and expensive elements [14]. These applications highlight the framework's versatility and relevance to global sustainability challenges.

5. Challenges and Limitations

Despite its promise, AI-driven materials discovery faces several challenges. Limited availability of high-quality experimental data restricts model generalization. Model interpretability remains critical for gaining trust among domain experts [15]. Additionally, integration with laboratory automation and standardized validation protocols is still evolving.

6. Future Directions

Future research should focus on integrating physics-informed learning, improving explainable AI techniques, and expanding open materials datasets. Hybrid approaches combining AI with high-throughput experimentation and digital twins are expected to further accelerate sustainable materials innovation [16].

7. Conclusion

This study presents a comprehensive AI-driven framework for accelerated materials discovery tailored to energy and sustainability applications. By integrating data-driven modeling, iterative validation, and real-world deployment, the framework addresses key limitations of traditional materials research. The results underscore AI's potential to transform sustainable materials development and support global energy transition efforts.

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