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Deep Learning-Driven Materials Informatics and Computational Modeling for Advanced Physical Systems

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Abstract

Deep learning-driven materials informatics has emerged as a transformative paradigm in the field of computational materials science, enabling accelerated discovery, design, and optimization of advanced materials for complex physical systems. The integration of data-driven methodologies with traditional computational modeling techniques has significantly enhanced the capability to predict material properties, analyze structure–property relationships, and simulate material behavior across multiple scales. This chapter presents a comprehensive overview of deep learning architectures and hybrid modeling frameworks that facilitate efficient exploration of high-dimensional materials design spaces. Emphasis is placed on the role of neural network models in materials property prediction, generative design, and real-time simulation of material systems under varying environmental and operational conditions. The coupling of physics-based models with deep learning approaches, including physics-informed neural networks and surrogate modeling techniques, enables improved accuracy while reducing computational cost associated with conventional simulation methods such as density functional theory and molecular dynamics. Applications in advanced physical systems, including energy storage materials, nanostructured systems, and high-performance engineering materials, demonstrate the potential of these approaches in addressing critical challenges in modern materials engineering. Persistent challenges such as data scarcity, model interpretability, and cross-domain generalization are also examined, highlighting the need for robust and scalable learning frameworks. The chapter underscores the growing importance of integrating artificial intelligence with materials science to establish autonomous and intelligent material discovery platforms.

Keywords: Materials Informatics, Deep Learning, Computational Modeling, Physics-Informed Neural Networks, Materials Property Prediction, Hybrid Simulation Models.

Introduction

Deep learning-driven materials informatics has emerged as a transformative direction in computational materials science, reshaping the manner in which materials are discovered, characterized, and optimized for advanced physical systems [1]. The increasing complexity of modern engineering applications, including energy storage devices, aerospace structures, and multifunctional nanomaterials, has created a demand for predictive frameworks capable of

handling large-scale, high-dimensional datasets [2]. Traditional experimental and simulation-driven approaches often struggle to efficiently explore the vast chemical and structural space of materials due to inherent limitations in time, cost, and scalability [3]. In response to these challenges, data-centric methodologies supported by deep learning have enabled systematic extraction of structure–property relationships from heterogeneous datasets derived from experiments [4], simulations, and high-throughput screening techniques. This paradigm shift has positioned materials informatics as a central component in next-generation materials design strategies [5].

The foundation of materials informatics lies in the integration of computational modeling with data-driven learning algorithms that can uncover hidden patterns within complex material systems [6]. Deep learning architectures such as convolutional neural networks, recurrent neural networks, graph neural networks, and transformer-based models have demonstrated strong capability in learning hierarchical representations of atomic and molecular structures [7]. These models facilitate prediction of mechanical, thermal, electrical, and electrochemical properties with high accuracy by capturing nonlinear dependencies that are often inaccessible through conventional analytical approaches [8]. The ability of deep learning systems to generalize from large datasets enables efficient exploration of unknown material spaces, thereby reducing reliance on exhaustive experimental validation [9]. This computational advantage has significantly accelerated the pace of innovation in materials science, particularly in the context of functional and structural materials [10].

Computational modeling techniques have long served as essential tools for understanding material behavior at different length and time scales [11]. Methods such as density functional theory, molecular dynamics simulations, and finite element analysis provide fundamental insights into atomic-level interactions, microstructural evolution, and macroscopic performance characteristics [12]. The computational cost associated with high-fidelity simulations restricts their applicability in large-scale material screening and real-time prediction scenarios [13]. The integration of deep learning with these physics-based models introduces a hybrid computational framework that enhances predictive efficiency while preserving physical interpretability [14]. Surrogate modeling approaches enable rapid approximation of complex simulations, allowing researchers to perform large-scale parameter exploration without compromising accuracy. This synergy between data-driven and physics-based methodologies represents a significant advancement in computational materials science [15].