Dissertation Summary

Recent progress in advanced materials science, manufacturing processes, and technological applications is driven by six key enabling technologies (KETs), which foster innovation, enhance industrial competitiveness, and drive progress across diverse sectors, from aerospace to healthcare, while promoting resilience and sustainability. This thesis aligns with four KETs identified by the European Commission, exploring the integration of advanced manufacturing, advanced materials, micro/nano-electronics, and artificial intelligence (AI) within the framework of Industry 4.0. Advanced manufacturing enhances production efficiency and customization through digitalization, enabling real-time process optimization and the development of high-performance materials and components. In parallel, advanced materials facilitate the creation of substances with tailored properties at the nano and atomic scale, promoting sustainable solutions through smarter production processes. Micro- and nano-electronics drive further technological progress by supporting the miniaturization of electronic components and improving computational efficiency. Central to these transformations is AI, which accelerates material discovery, optimizes production workflows, enhances predictive modelling across multiple scales, and facilitates automation in advanced manufacturing environments.

In this context, the primary objective of this research is to leverage AI-driven methodologies to accelerate the discovery and optimization of innovative materials. Conventional atomistic simulations, while accurate, often suffer from high computational costs, making them impractical for large-scale problems. To overcome this limitation, the dissertation introduces data-driven approaches that combine predictive modelling with efficient material representations. A key challenge addressed in this work is developing scalable representations for complex nanostructured systems, particularly graphene-based, two-dimensional (2D) and quasi-2D materials. These representations are essential for connecting AI and advanced materials, as they encode structural features into formats suitable for accurate prediction tasks, ensuring computational efficiency and unlocking the full potential of AI-driven materials discovery and automated workflows. A significant focus is placed on image-based representations for defect-rich materials, which enable the integration of geometric and chemical features into machine learning (ML) models. To validate the proposed methodologies, robust datasets were generated by combining atomistic simulations, such as Density Functional Tight Binding (DFTB), performed through an automated workflow for geometry optimization and property calculation, with synthetic data created using variational autoencoders (VAEs).

The dissertation also seeks to address the multiscale nature of material behavior by establishing methodologies that connect nanoscale structural features to macroscale properties. This entails developing models capable of correlating intrinsic material properties with key production parameters, ultimately allowing for the prediction of the mechanical properties of final products. A practical application of this approach involves predicting the mechanical properties of 3D-printed specimens by combining material properties with printing parameters. This work, conducted in collaboration with the Innovation Centre of the Faculty of Mechanical Engineering in Belgrade as part of the EuMINe COST Action (CA22143), demonstrates the potential of AI-driven frameworks for optimizing additive manufacturing (AM) processes.

The structure of the thesis is designed to reflect a logical progression from fundamental concepts to the development of novel methodologies, culminating in their practical application to real-world problems in advanced materials science. The initial chapters provide background information on nanomaterials and 2D materials, with a focus on graphene-based materials, establishing the foundation for understanding their unique properties and challenges. This background is followed by a detailed exploration of AI methodologies, including convolutional neural networks (CNNs), graph neural networks (GNNs), boosting algorithms, transformers, and VAEs. A dedicated chapter focuses on material representations in AI, emphasizing their critical role in connecting advanced materials and AI through robust encodings of geometric and structural properties that enable predictive modelling and high-throughput screening.

Building upon these methodologies, this dissertation introduces GrapheNet, a novel image-based representation framework for nanographene flakes. Unlike conventional approaches, GrapheNet encodes spatial information directly into images, enabling accurate property prediction through CNNs. This framework enhances computational efficiency and scalability, demonstrating superior performance compared to state-of-the-art methods.

Expanding on this framework, the dissertation presents a comprehensive defect characterization methodology for graphene nanoflakes. This approach employs object detection and feature extraction techniques to analyze defects, integrating ML models such as XGBoost with frequency- and geometric-domain features. Moreover, a novel synthetic data generation approach using VAEs is introduced to expand the applicability of the defect detection framework. This VAE facilitates the generation of synthetic datasets of defected nanoflakes with target structures, particularly optimized for applications in nano-electronic devices.

These ML methodologies were further adapted for macro-scale applications, such as predicting the mechanical properties of polymeric specimens produced via AM. An integrated framework combines experimental data from tensile tests with ML models, achieving strong predictive performance for mechanical elastic properties. Furthermore, the framework enhances model explainability by identifying the features that have the greatest impact on mechanical behavior.

To conclude, this thesis demonstrates how cutting-edge AI-driven methodologies can revolutionize advanced materials science by providing scalable, accurate, and efficient solutions to long-standing challenges. The presented frameworks and models connect theoretical research with real-world applications, driving innovation in fields such as nanotechnology, AM, and sustainable materials development. These advancements align with the vision of Industry 4.0, where the convergence of AI, advanced materials, and smart manufacturing processes is essential for achieving fully digitalized and automated production environments, driven by seamless workflows and intelligent decision-making systems. While this dissertation lays the foundation for several advancements, future research directions open to further exploration include enhancing the scalability of the proposed methods, improving data integration from heterogeneous sources, and extending the applicability of the frameworks to other classes of advanced materials and manufacturing techniques.