JAPAN ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY

Abstract

Co-Creative Intelligence research area
School of Knowledge Science

Knowledge science

AI development for capturing dynamic phenomena in materials: Insights and innovation through Deep learning model design and application

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This dissertation presents a domain-enriched deep learning framework for representation learning in materials science, addressing the challenges of capturing the complexity of dynamic, multidimensional material data where traditional descriptors are often insufficient. By embedding materials science knowledge within deep learning models, this research advances representation learning to support both predictive accuracy and scientific insight. The framework is applied to two key scenarios. First, in an unsupervised setting, it learns representations to reconstruct material images, capturing hidden structures and evolving patterns within the data and enabling discovery of material dynamic behaviors. Second, in a supervised learning context, it develops representations to predict material properties achieving both high accuracy and interpretability about structure-property relationship. This work highlights the impact of domain-guided representation learning, bridging deep learning with scientific principles to advance material discovery. Through case studies, it demonstrates that domain-enriched deep learning is not merely predictive but instrumental in generating insights, offering a versatile approach that strengthens the role of data-driven models in materials science innovation.

Keywords: Materials discovery, Data-driven approach, Deep Learning, Physics-informed, Materials Property, Materials Imaging