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論文題目	AI development for capturing dynamic phenomena in materials: Insights and innovation through Deep learning model design and application
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論文の内容の要旨

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

論文審査の結果の要旨

Analyzing and understanding dynamic phenomena in materials is challenging and multifaceted, requiring both precise measurements and accurate interpretations. While traditional analytical methods have been valuable, they face limitations in capturing complex dynamic behaviors and predicting material properties. This doctoral thesis addresses these limitations by developing innovative deep learning frameworks that integrate domain knowledge for enhanced material analysis and property prediction.

The thesis focuses on two key scenarios: unsupervised learning for dynamic imaging and supervised learning for property prediction. For dynamic imaging, the PID3Net framework was developed to reconstruct material structures from X-ray diffraction patterns, incorporating physics principles and temporal constraints to achieve high-quality imaging of moving nanoparticles. For property prediction, the SCANN framework employs self-consistent attention mechanisms to analyze material structures at both local and global scales, enabling accurate prediction of material properties while providing interpretable insights into structure-property relationships.

The thesis demonstrates the effectiveness of combining domain expertise with modern AI techniques, particularly in scenarios where data might be limited but scientific knowledge is rich. This integration enables more accurate analysis and prediction while maintaining interpretability, crucial for scientific applications. The work has been recognized through 2 publications in *npj Computational Materials* (a journal in Nature Portfolio; top 1% in Mathematics/Modeling and Simulation, and top 5% in Computer Science/Computer Science Applications), highlighting its significant contribution to the field.

This is an outstanding dissertation, and we approve awarding a doctoral degree to Mr. VU Tien Sinh.