Automated Atomic Scale STEM Data Analysis and Modelling for Energy Materials

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The discovery, optimization, and application of new materials is a complex and multifaceted process that encompasses identifying technological needs, reviewing existing literature, proposing candidate materials, engineering devices, characterizing structures, and testing performance. This workflow becomes particularly time-consuming and costly when atomic-level precision is required to understand the functionality of materials and heterostructured devices.
To address these challenges, we introduce an AI-enhanced analytical workflow based on machine learning and deep learning techniques that automate the analysis of transmission electron microscopy (TEM) data. This workflow enables comprehensive characterization of materials and device architectures, with a focus on energy and environmental applications, as well as quantum materials and their associated heterostructures.
Our pioneering workflow autonomously identifies material composition, crystallographic phases, and spatial orientations across diverse regions of (S)TEM images and datasets through advanced model comparison. It also incorporates automated strain analysis, offering a detailed understanding of structural properties. The extracted data is used to generate 3D atomic and finite element models, which facilitate theoretical simulations and provide critical physical and chemical insights into device performance under real-world conditions.
This methodology is highly versatile and demonstrates strong generalization capabilities across different material systems. Beyond addressing the urgent need for automation in materials characterization, it enables the generation of accurate physical models and simulations of complex devices with unprecedented precision. [1-3]

References

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