Unlocking Twisted 2D Materials: A Nanoscale Exploration of Bandgap Dynamics

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The unique sensitivity of local electronic properties in two-dimensional (2D) materials, such as their bandgap, to the underlying crystal arrangements provide exciting prospects for novel quantum nano-optoelectronic applications [1,2]. However, the limitations of current characterization techniques in accessing this delicate relationship with nanoscale resolution have made it challenging to understand the impact of local structural phenomena such as strain, thickness, and layer rotation on electronic properties. Here, we present a comprehensive strategy for determining the relationship between bandgap energy and local thickness and strain fields in twisted van der Waals materials. Unveiling these structure/property correlations is crucial for gaining a complete understanding of the rich bandgap dynamics at the nanoscale in these materials. By combining advanced techniques such as electron energy-loss spectroscopy assisted with machine learning [3] and 4D scanning transmission electron microscopy with an Electron Microscopy Pixel Array Detector, we evaluate the bandgap and local strain fields in twisted WS₂ with nanoscale resolution. We demonstrate how strain can increase the bandgap by up to 30% in regions with significant twist angles between layers and hence pronounced local strain fields (Figure 1). This approach provides a flexible tool for uncovering the connection between strain and bandgap dynamics in 2D materials and can also be applied to more complex 2D material geometries and heterostructures, contributing to the development of novel technologies for quantum devices.

References


Figures

Figure 1: Visualization of the Interplay between Local Thickness and Bandgap Energy in a Twisted WS₂ flake: (inset) Strain Map of the \( \mathbf{e}_x \) Component.