Strain-Driven Bandgap Increase in Twisted 2D Quantum Materials: A Nanoscale Study

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Twisted two-dimensional materials offer a unique platform to realise novel quantum nano-optoelectronics applications thanks to the sensitivity of their local electronic properties with respect to their underlying crystal atomic arrangements [1-4]. However, the limitations of existing techniques to access this subtle structure/property interplay with nanoscale resolution have made it challenging to disentangle the effects that variations in local strain, thickness, and rotation angle between layers have on their electronic properties. Here we present a novel strategy for determining the dependence of the bandgap energy on local thickness and strain fields in twisted van der Waals materials. This is an essential step towards a quantitative understanding of bandgap dynamics at the nanoscale in these materials. By combining electron energy-loss spectroscopy boosted by machine learning [5,6] and 4D scanning transmission electron microscopy using an Electron Microscopy Pixel Array Detector, we evaluated the bandgap and local strain fields in twisted WS_2 with nanoscale resolution. Our findings indicate that the bandgap energy can increase by up to a factor of 30% in regions characterised by sizeable twist angles between layers and hence by marked local strain fields (Figure 1). Our approach provides a novel toolbox in our quest to unveil the relationship between strain and bandgap dynamics in 2D materials. Furthermore, it can also be applied to more complex 2D materials geometries and heterostructures, as required for the development of novel technologies for quantum devices.

References

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Figures

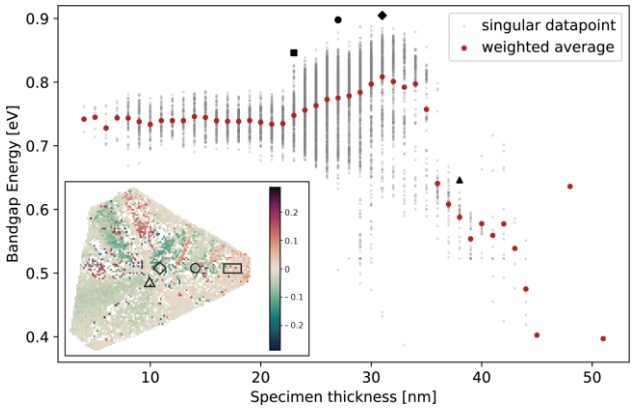

Figure 1: Visualisation of the relation between the specimen thickness and bandgap energy in a twisted WS_2 flake. (inset) local strain map of the ε_{xy} component on the same twisted flake.