Automatic detection of W vacancies in WS_2 through CNN

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Two-dimensional (2D) materials, such as WS2, have garnered significant attention for their potential applications in quantum computing and related technologies. These materials exhibit unique electronic and optical properties owing to their atomically thin nature and strong quantum confinement effects. In particular, vacancies, or defects, within these materials play a pivotal role in influencing their quantum behaviour [1].

Vacancies introduce localized electronic states within the bandgap of 2D materials, altering their electronic structure and optical properties. These defect-induced states can serve as quantum emitters, enabling applications in single-photon sources, quantum communication, and quantum information processing [2].

Understanding and controlling vacancies in 2D materials are thus essential for harnessing their full potential in quantum technologies. High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy (HAADF-STEM) emerges as a powerful technique for probing the atomic-scale structure of 2D materials like WS2, allowing precise characterization of vacancies and their effects on the material's quantum properties [3].

In this study, we present an automated method for identifying vacancies in WS2 monolayers. Our approach leverages a convolutional neural network (CNN) for denoising, applied to Fast Fourier Transform (FFT) spectra. The CNN model is trained on a dataset comprising over 5000 simulated spectra [4, 5]. By filling in the gaps corresponding to vacancies, this denoising technique facilitates accurate tracking of vacancy locations through image differencing.

Our work underscores the importance of vacancies in 2D materials for quantum applications and highlights the significance of advanced imaging techniques like HAADF-STEM in studying quantum materials at the atomic level. This automated detection method paves the way for further exploration and utilization of vacancies in WS2 and other 2D materials for quantum technologies.

References

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Figures

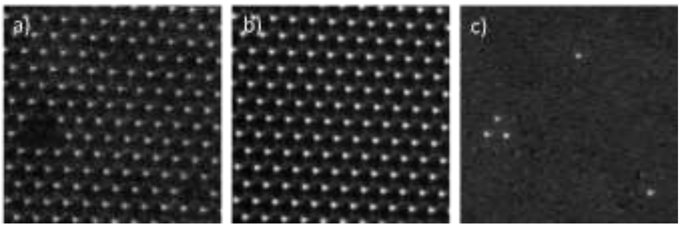

Figure 1: a) HAADF-STEM image of WS2 material with vacancies. b) Image with vacancies refilled. This image was obtained through FFT denoising using CNN. c) Image showing vacancy positions.