

Automatic detection of vacancies in WS₂ for Quantum Materials studies using HAADF-STEM Imaging

Ivan Pinto-Huguet^a

Marc Botifoll^a, Jordi Arbiol^{a,b}

a. Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Barcelona, Catalonia, Spain

b. ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Catalonia, Spain

ivan.pinto@icn2.cat

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

- [1] Liu X., Hersam M.C., *Nat Rev Mater*, 4 (2019) 669-684
- [2] Parto K., Azzam S.I., Banerjee K. et al., *Nat Commun*, 12 (2021) 3585
- [3] Sytze de Graaf and Bart J Kooi, *2D Mater.* 9 (2022) 015009
- [4] Ziatdinov M., Dyck O., Maksov A. et al., *ACS Nano*, 11, 12 (2017) 12742–12752
- [5] Botifoll M., Pinto-Huguet I., Arbiol J., *Nanoscale Horiz.*, 7 (2022) 1427-1477

Figures

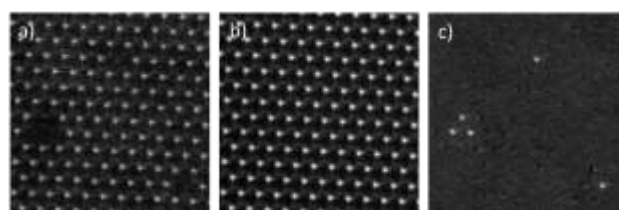


Figure 1: a) HAADF-STEM image of WS₂ material with vacancies. b) Image with vacancies refilled. This image was obtained through FFT denoising using CNN. c) Image showing vacancy positions.