Defect Implementation in 2D vdW Materials: Highly Correlated Fermion States and Autonomous Experimentation

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Defects within two-dimensional materials, such as transition metal dichalcogenides, enable a path to engineer new material functionality beyond conventional doping schemes. Chalcogen vacancies (0D) and mirror twin boundaries (1D) can be created at controllable densities to provide reactive sites for subsequent functionalization and the visualization of exotic phenomena such as the presence of quantum fluids in WS_2 [1]. The investigation of these systems with cross-correlative measurements that combine nano angle-resolved photoemission spectroscopy and scanning probe microscopy will be presented. Additionally, the usage of convolutional neural networks and Gaussian processes enables the direction of autonomous experimentation without the need of a human operator [2]. The implementation of a machine-driven workflow for hyperspectral tunnelling spectroscopy will also be discussed.

References

[1] Rossi, A., Thomas, J. C. et al. arXiv:2301.02721 (2023)
[2] Thomas, J. C., Rossi, A. et al. npj Comput. Mater. 8, 99 (2022)

Figures

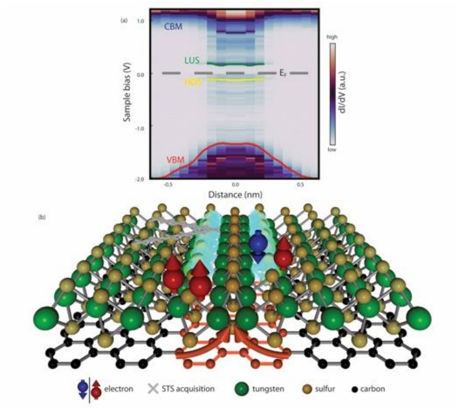

Figure 1: Band gap renormalization over a 1D defect within WS_2 realized at the atomic scale.

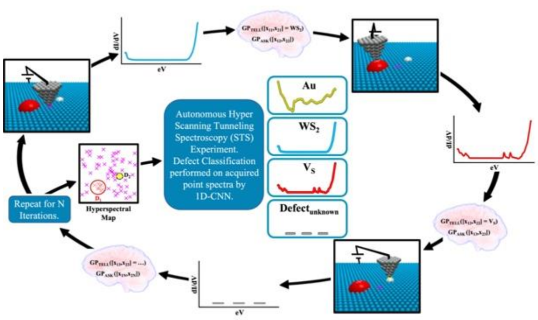

Figure 2: Hyperspectral data collection using a machine-driven workflow across a substrate accessible with a scanning tunnelling microscopy.