

# Classification of Atomic Defects in Semiconductor Material Systems by Machine Learning

Calvin Pei Yu WONG<sup>1</sup> and Kuan Eng Johnson GOH<sup>1, 2, 3</sup>

<sup>1</sup> *Institute of Materials Research and Engineering (IMRE), Agency for Science Technology and Research (A\*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634*

<sup>2</sup> *Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117551*

<sup>3</sup> *Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798*

[calvin\\_wong@imre.a-star.edu.sg](mailto:calvin_wong@imre.a-star.edu.sg), [gohj@imre.a-star.edu.sg](mailto:gohj@imre.a-star.edu.sg), [kejgoh@yahoo.com](mailto:kejgoh@yahoo.com)

Visualizing and identifying defects present on the semiconductor material surface is an important application of the scanning tunnelling microscope (STM). However, it can be difficult to interpret these images as the images show a convoluted picture of the local electronic structure and topography. Identifying the correct defect require comparisons to theoretical predictions and is often highly dependent on the skill of human experts. Thus, the identification of a large dataset is not only time consuming but may also result in inconsistency in the classification of experimental STM images due to human bias. In this work, we compare the performance of a convolutional neural network (CNN) trained solely using theoretical simulated defect images with human classifiers and discuss the implications of our results.