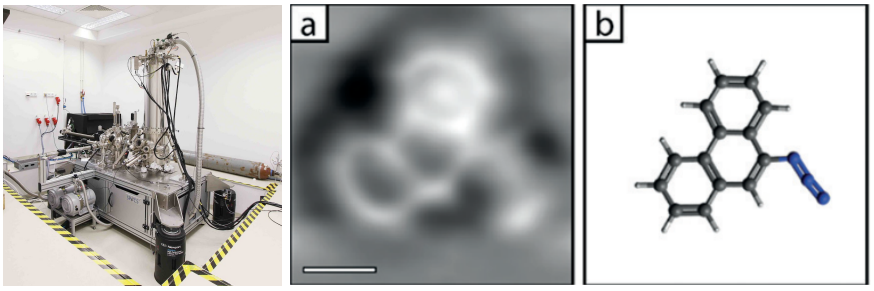
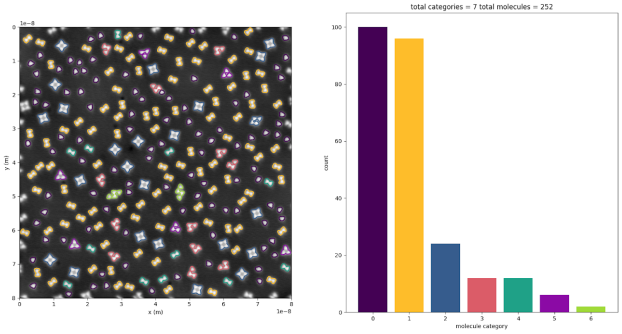
ADS1001 data challenges 1 https://handbook.monash.edu/current/units/ADS1001
Dr Simon Clarke

Project: “Counting Molecules”
Jack Hellerstedt, Physics, Monash
Tyler Hennen, EE, RWTH Aachen

Scanning tunneling microscopy (STM; instrument photo below) is the experimental technique made famous in the 1980’s at IBM for achieving atomic resolution [1, 2]. In addition to atoms, innovations of this technique make it possible to resolve chemical bonds, making it possible to “take a picture of a molecule” (example below) [3].



This project will use the imaging data available from these techniques, and leverage the machine learning software libraries built using python (scikit-learn), to refine an algorithm to automate the counting and sorting of different molecule species. An example of the current state of this algorithm can be seen below (compare to the hand-counted version [4]).



The students working on this project will use the existing code-base as a way to familiarise themselves with python, scientific computing libraries (scipy, numpy, scikit-learn), github version control, and make progress towards visualising “molecular fingerprints” to understand and refine how to automate the categorisation of different molecular species.

References:

1. The Nobel Prize in Physics 1986. NobelPrize.org. Nobel Media AB 2020. Thu. 7 May 2020. <https://www.nobelprize.org/prizes/physics/1986/summary/>
2. Binnig, G., Rohrer, H., Gerber, C., & Weibel, E. (1982). Surface Studies by Scanning Tunneling Microscopy. *Physical Review Letters*, *49*(1), 57–61. https://doi.org/10.1103/PhysRevLett.49.57
3. Jelínek, P. (2017). High resolution SPM imaging of organic molecules with functionalized tips. *Journal of Physics: Condensed Matter*, *29*(34), 343002. https://doi.org/10.1088/1361-648X/aa76c7
4. Stetsovych, O., Švec, M., Vacek, J., Chocholoušová, J. V., Jančařík, A., Rybáček, J., … Starý, I. (2016). From helical to planar chirality by on-surface chemistry. *Nature Chemistry*, *9*(3), 213–218. https://doi.org/10.1038/nchem.2662