Defect Engineering within Transition Metal Dichalcogenides and Machine Learning Approaches towards STM/STS Tip Shaping on Au

J. C. Thomas, K. Cochrane, and A. Weber-Bargioni

Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

Monolayer transition metal dichalcogenides (TMDs), such as WS_2 and WSe_2, have gained substantial interest for point-defect control, serving as host substrates for quantum emitters, exhibiting spin-valley splitting properties, and showing capability towards tunable band gap engineering. Sulfur vacancies can be controllably created to serve as target sites for photo- and spin- active functionalization [*e.g.*, decorated cobalt or rare-earth atoms in TMDs]. Scanning probe microscopy (held in ultra-high vacuum and low temperature) can measure the electronic characteristics at the atomic level of induced defects, while also providing a path to excite single-defect optical transitions. Here, we delve into filling defect vacancies in synthetic host TMD materials to enable investigations in localized photon emission, determine spin-orbit interaction, and identify subsequent band structure with scanning probe microscopy and spectroscopy.

In situ tip treatment and classification is crucial to obtaining high quality scanning tunneling micrographs. We use machine learning (ML) techniques on Au {111} substrates to identify herringbone structure, double tips, and step edges using an automated approach that feeds into a ML controlled tip-shaping program. Feature extraction techniques in both real and Fourier space provide dimensionally reduced input that also minimize training computation cost; comparisons across common artificial intelligence approaches are presented.