Defects fingerprints in single layer MoS_2 by *ab initio*-based STM and AFM simulations

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Defects can dramatically modify the performance of 2D-based devices. In the case of MoS_2, many of these defects have already been observed, both point-like [1] and extended [2]. However, with the exception of the S monovacancy, a detailed characterization of their electronic, magnetic and transport features is still lacking.

A valuable tool for identifying the properties of such defects is Scanning Probe Microscopy (SPM). However, the interpretation of the images produced *via* this technique is not always straightforward and often requires the help of atomic-scale simulations to provide a correct understanding of the sample under study.

We present an *ab initio* study of the most common point-like defects observed in monolayer MoS_2. We analyze their electronic and transport features of the selected defects and supply their simulated images for both the Scanning Tunneling (ST) [3] and Atomic Force (AF) [4] Microscopy techniques.

Our results show the strong dependence of the STM image contrast behavior on the metallic or semiconducting character of the defects, and the influence of the tip nature and its reactivity on the image pattern obtained with the AFM, thus providing a valuable tool to interpret experimental results.

References

[1] J. Hong et al. Nature Communications 6 (2015) 6293
[2] Y.L. Huang et al. Nature Communications 6 (2015) 6298
[3] C. González, B. Biel and Y. Dappe, Nanotechnology 27 (2016) 05702 (2016)
[4] C. González, Y. Dappe and B. Biel The Journal of Physical Chemistry C 120 (2016) 17115

Figures

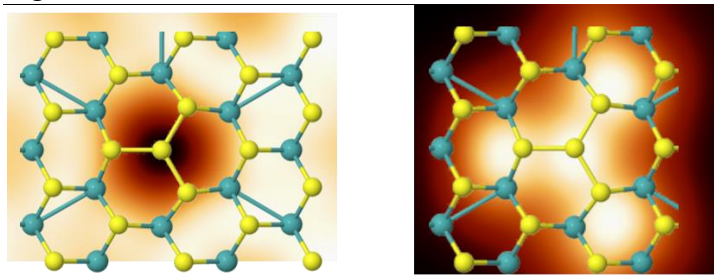

Figure 1: Simulated STM images of a Mo monovacancy with two substitutional S atoms at voltages V = +1.9 V (left) and V = +0.5 V (right)

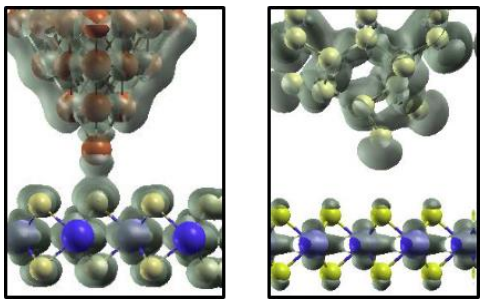

Figure 2: Charge distribution at the most attractive point between the MoS_2 monolayer and a Cu (left) and Si (right) tips