Defect Fingerprints and Reactivity by Ab Initio-based STM and AFM Simulations in Single Layer MoS2

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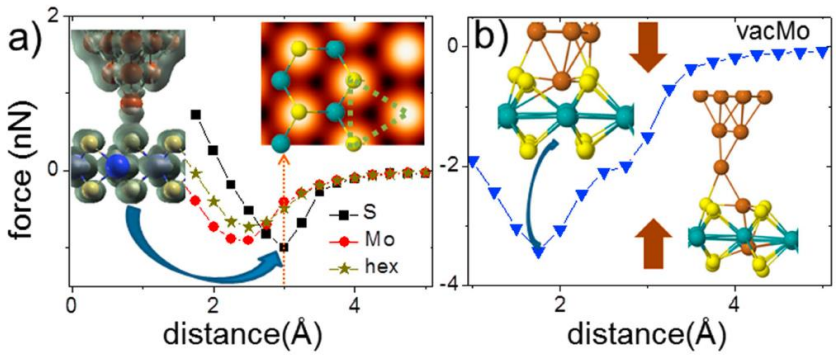
Defects [1] and dopants [2] can dramatically modify the electronic and transport properties of low-dimensional materials such as graphene and other members of the two-dimensional (2D) family. We provide an exhaustive first-principles characterization of the most common point-like defects occurring during the growth process in a MoS2 monolayer (namely S and Mo vacancies, di-vacancies, and their corresponding substitutional antisites). In addition to the analysis of the defect-induced modification of the structural, electronic and magnetic properties of the MoS2 monolayer, we performed ab initio-based simulations of both Scanning Tunneling (STM) [3] and Atomic Force Microscope (AFM) [4] images for every defect, showing that the interpretation of the defects images must take into account the delicate interplay between geometric and electronic effects taking place between sample and tip. Furthermore, we show how the electronic character of the probe tip (semiconducting or metallic) is critical to understand the physical origin of the obtained AFM curves, which can ultimately be explained in terms of a simple model of the metal-semiconductor junction formed between the metallic tip and the semiconducting-like defects, or vice-versa. Finally, we demonstrate the enhanced reactivity of the MoS2 monolayer in the presence of certain defects and the possibility of tuning its electronic properties for molecular sensing by locally modifying the electronic environment by means of atomic doping by AFM manipulation.

[1] C. Gómez-Navarro, P. J. de Pablo, J. Gómez-Herrero, B. Biel, F. J. García-Vidal, A. Rubio and F. Flores, Nature Materials 4, 534 (2005)

[2] B. Biel, X. Blase, F, Triozon and Stephan Roche, Physical Review Letters 102, 096803 (2009); B. Biel, F, Triozon, X. Blase and Stephan Roche, Nano Letters 9, 2725 (2009)

[3] C. González, B. Biel and Y. Dappe, Nanotechnology 27, 105702 (2016)

[4] C. González, Y. Dappe and B. Biel (submitted)



a) Cu-S bond formed on an tip-MoS2 contact, the AFM pattern is induced by the force values; b) Reactivity enhancement on a Mo-vacancy and apex trapping after retraction.