Point-like defects in transition metal dichalcogenides characterized by SPM simulations

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Defects are frequently present in 2D materials, and as such have been extensively studied on suspended samples. However, to describe realistically their electronic properties and their SPM characterization, simulations need to take into account the presence of the metallic substrates commonly employed during the growth and the characterization processes, which might substantially alter the electronic structure of the 2D material.

The interaction between metallic substrates and pristine transition metal dichalcogenides (TMDs) can greatly vary depending on the metal [1]. In this work, we have studied the interaction of several point-like defects in TMDs monolayers with underneath Ir(111) and Au(111) substrates by means of DFT calculations and SPM simulations, revealing a notably different behavior depending on the metallic substrate considered. The hybridization of the S states with those of the Ir(111) substrate induces a shift of ~1 eV of the MoS_2 states towards the valence band and a large broadening of the defect states [2]. The interaction with a gold substrate is much weaker, as confirmed by experimental data [3], leading to sharper defect states (Fig.1), much more similar to those found for freestanding MoS_2.

References

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[2] I. Delac Marion, D. Capeta, B. Pielic, F. Faraguna, A. Gallardo, P. Pou, B. Biel, N. Vujicic and M. Kralj, Nanotechnology, 29 (2018) 305703.

[3] N. Krane, Ch. Lotze, P. Pou, B. Biel and K. Franke (in preparation)

Figures

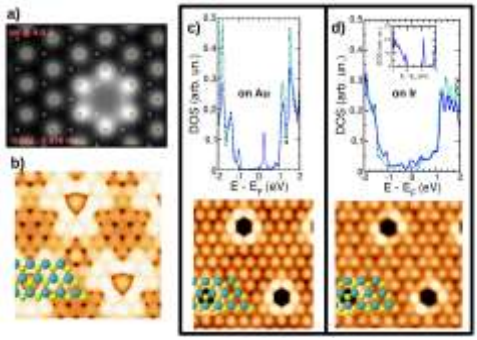

Figure 1: Left panel: AFM (a) and STM at -0.1 V (b) images of a S vacancy at the top layer for freestanding MoS_2. Right panel: LDOS of top S atoms close (blue) and far (cyan) of the defect site and STM images at V = -0.1 V for a top S vacancy in epitaxial MoS_2/Au(111) (c) and MoS_2/Ir(111) (d). Inset in d): LDOS of a top S vacancy in freestanding MoS_2.