Chemical Characterization of MoS2 using Theoretical AFM

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Abstract

Since graphene was discovered some years ago [1], the interest for two dimensional (2D) materials has grown exponentially. The so-called transition-metal dichalcogenide (MX2) have recently attracted a great attention due to their promising properties. One of the most studied MX2 compounds is the MoS2 due to its semiconducting character and its possible nanoelectronic, optoelectronic and spintronic applications [2]. This material has been studied with different techniques but a complete atomic force microscopy analysis (AFM) cannot be found in the literature.

In this work, we have performed density functional theory (DFT) simulations based in the VASP code [3] in order to present a detailed AFM analysis of a perfect MoS2 monolayer (together with its most characteristic defects) using different tips: a low/high interacting Si/Cu tip and the recently developed stable C-based tip [4]. Our results allow us to identify the different defect presented in a MoS2 monolayer, confirming the higher chemical interaction obtained when any atomic vacancy is examined. As expected, the metallic tip presents the highest interaction. Finally, the graphitic tip shows the lowest reactivity and a great stability, even when the van der Waals (vdW) forces are included in the calculation. This result confirms the graphitic tip as adequate for AFM measurements, especially with highly reactive systems where the atomic transfer is undesirable and it can be expected with other tips.

CG acknowledges funding from Andalusian Agency of Knowledge and the 7th Framework Programme via the Marie Curie Action, “Co-funding of Regional, National and International Programmes” through the Andalucia Talent Hub grant.

References

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Figures

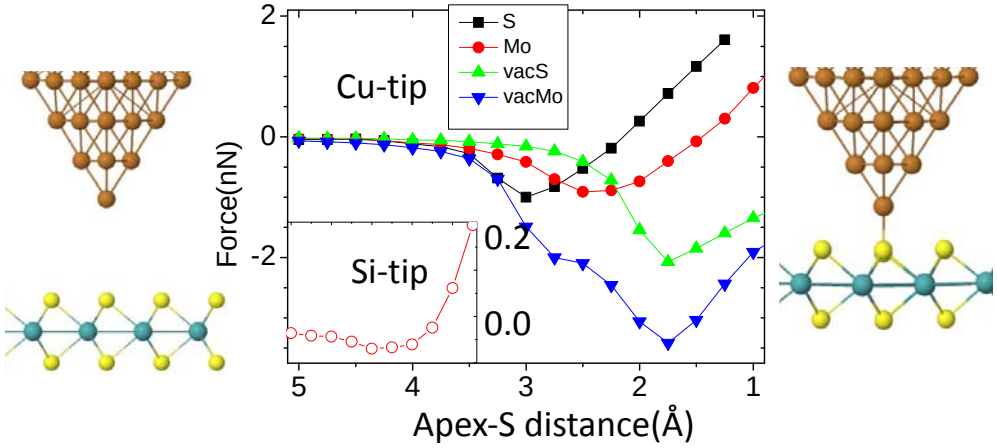

Figure 1: Schematic representation of a Cu tip over a S atom in the MoS2 monolayer for long distance and in the contact regime together with the force curves obtained over the S and Mo atoms and their corresponding vacancies. In the inset, the same result obtained over a Mo atom using a low interacting Si-tip.