Detection of Inorganic Molecules on reactive MoS_2 defects by *ab-initio* Atomic Force Microscopy Simulations

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Abstract

Since graphene was discovered some years ago [1], the interest in two dimensional (2D) materials has grown exponentially. The so-called transition-metal dichalcogenides have recently attracted a great attention due to their promising properties. One of the most studied compounds is the MoS_2 due to its potential nanoelectronic, optoelectronic and spintronic applications [2]. Very recently, this material has been proposed as a fundamental part in gas sensors [3]. In those cases, the molecules were weekly bonded by van der Waals (vdW) forces to the poorly reactive MoS_2 substrate, changing the electric current measured in the sensor.
In this work, we have performed density functional theory (DFT) simulations based in the VASP code [4] in order to find the most stable structures of small inorganic molecules (such as H_2O, NO and CO_2) adsorbed on different point defects of the MoS_2 monolayer [5]. Our results show that the molecules can be bonded to the Mo atoms in the substitutional defects. In our analysis, the Sulphur divacancy occupied by two Mo atoms has been selected as the most interesting defect. Once the molecules are absorbed over this point, they can be identified using an atomic force microscope (AFM). Following the original idea of chemical identification proposed some years ago [6], each molecule will lead to a different force curve when an AFM tip is approached. In figure 1, the forces of H_2O, NO and CO_2 molecules are represented. The resulting value and position of the minimum force characterize the kind of molecule that has been scanned by the AFM. Finally, a comparison between a reactive metallic tip and a low reactive Si tip will define the best option for future experimental measurements.

References

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Figure

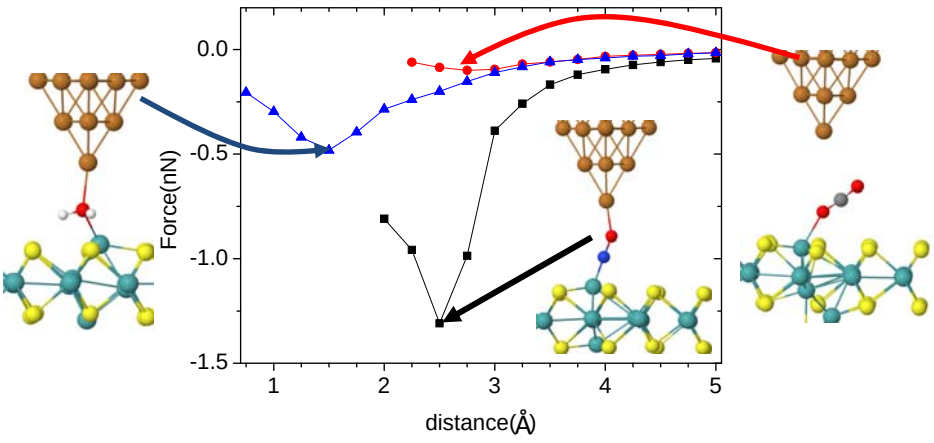

Figure 1. Force curves of a Cu tip contacting to three different molecules adsorbed on a defect formed by the substitution of two S by two Mo atoms in the MoS2 monolayer. The ball and stick models of the contact point (minimum force) are shown: on the left side, a H2O molecule (blue triangles), on the right side a CO2 molecule (red circles) and on the inset a NO molecule (black squares).