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First-Principles Simulations of Vacancies and Grain Boundaries in Monolayer MoS_2-Au Interfaces for Unconventional Computing Paradigm

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Abstract
Atomically thin two-dimensional (2D) materials have been —and are still currently being— extensively studied due to their desirable mechanical, electronic, and optical properties. These, together with the materials' intrinsic ultra-thin size, have the potential to enable the development of compact devices and innovative, beyond-CMOS, technologies.

Here we look at single-layer molybdenum disulphide (MoS_2) as the core material in 2D memristors for neuromorphic computing applications [1-3]. 2D memristors based on MoS_2 present several advantages with respect to conventional devices based on transition metal oxides: good flexibility, high transparency, and the potential to work when applying low voltages (0.1 - 0.2 V), thus allowing the fabrication of compact and energy-efficient devices. However, there is still much debate regarding the physics of their resistive switch, which is thought to depend on both surface defects and the type of metal-semiconductor junction [4]. Moreover, the metal contact is particularly important when designing such devices, as it can significantly influence the properties of MoS_2 at the interface. Indeed, both surface defects, which are intrinsically present in the material following common growing techniques such as CVD, and the nature of the metal contact affect not just the performance but also the working mechanism of 2D memristors.

To shed light onto the physics of metal-MoS_2 interfaces, we carry out atomistic computer simulations in the framework of density functional theory (DFT). We employ surface calculations based on the Green's function, in order to construct realistic interfaces and to compute surface properties. To model the metal electrode, we choose Au as it is commonly one of the most popular choices, and it has been successfully used to develop 2D memristors [4]. In this work, we want to bridge the gap between materials' properties and device physics and to do so, we investigate the impact of both experimentally-observed point defects (i.e., vacancies and substitutions) and extended defects, such as grain boundaries, on the physics and chemistry of Au-MoS_2 interfaces. To the best of our knowledge, this is the first attempt to thoroughly model interfaces in the presence of grain boundaries.

Ultimately, our study constitutes the first step of a more comprehensive multi-scale modelling approach, in which the aim is to construct a full atomistic-to-device level model that can aid us in elucidating the working mechanism of 2D memristors based on single-layer MoS_2.

[1] EU H2020 NeurONN Project, www.neuronn.eu.
[2] A. Todri-Sanial et al., *IEEE Trans. Neural Netw. Learn. Syst.*, 1-14, **2021**.
[3] A. Todri-Sanial, *MRS Fall Meeting and Exhibit*, **2021**.
[4] R. Ge et al., *Nano Lett.*, 18, 434-441, **2017**.

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