MoS_2 for Unconventional Computing and Biosensing Applications: A First Principles Study

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Atomically thin two-dimensional (2D) materials have been —and are still currently being— extensively studied due to their desirable mechanical, electrical, and optical properties, which enable the development of innovative devices and technologies. Within the vast chemical space of transition metal dichalcogenides (TMDs), single-layer molybdenum disulphide (MoS_2) is with no doubt one of the most studied material due to its stability and its direct optical band gap of 1.8 eV, which make it the ideal candidate to be used in a wide range of nanoelectronic devices, going beyond the conventional CMOS technology.

Here we look at MoS_2 in the context of two different cutting-edge applications: first, as the core material in 2D memristors for neuromorphic computing, and then as the sensing material in field-effect biosensors. We want to bridge the gap between materials' properties and device physics and to do so, we carry out atomistic computer simulations in the framework of density functional theory (DFT). We study a planar MoS_2 device that can be exploited either as a memristor device or field-effect biosensing device depending on its geometry.

2D memristors based on MoS_2 present several advantages with respect to conventional memristors based on transition metal oxides, such as 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.(1) 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.(2,3) The metal contact is particularly important when designing such devices, as it can significantly influence the properties of MoS_2 at the interface. Effectively, this could affect not just the performance, but also the working mechanism of 2D memristors. Thus, we investigate different metal/MoS_2 interfaces with the aim of better understanding the surface physics of such junctions. 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.

Recently, MoS_2 has also been studied as a sensing platform for detecting gas and small biological molecules, such as glucose.(4) Enzymatic biosensing is the most common approach, however, non-enzymatic sensing can provide higher sensor stability and prompt response at the expense of chemical selectivity. Here, we are interested in the non-enzymatic detection of cortisol in human sweat as a mean to monitor the risk of cardiovascular diseases. However, it is not known if such analyte interacts in a suitable way with MoS_2, and if so, how. Thus, we thoroughly explore the MoS_2/cortisol interaction in terms of both structural, electronic, and charge transfer properties to assess viable sensing mechanisms. We also study the impact of some of the most used metal dopants employed in lab-scale experiments, such as Ni, Pt, Pd, in order to modulate the sensing platform with respect to bare MoS_2.

Overall, our work ultimately aims to obtain a deep understanding of the properties of MoS_2 when used in different applications to drive the design of devices towards better performance.

References

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