Quantum Mechanical Simulations of 2D Materials for Unconventional Computing and Biosensing Applications

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Quantum mechanical simulations of 2D materials for unconventional computing and biosensing applications

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Atomically thin two-dimensional (2D) materials have been —and are still currently being— extensively studied due to their unique mechanical, electrical, and optical properties, which enable the development of innovative devices and technologies. Within the wide chemical space of transition metal dichalcogenides (TMDs), single-layer molybdenum disulphide (MoS_2) is with no doubt one of the most studied materials 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 conventional CMOS technology.

Here we look at MoS_2 in the context of two different cutting-edge applications: first, as the core material for 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 which, depending on its geometry, can be exploited either as a memristor device or field-effect biosensing device.

2D memristors based on MoS_2 present several advantages with respect to conventional memristors based on transition metal oxides, such as good flexibility, high transparence, 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] Monolayer-MoS_2 memristors ("atomristors") are technologically relevant, although there is still much debate regarding the physics of their resistive switch, which is thought to depend on both surface defects and on the type of metal-semiconductor junction.[2,3] To shed light on the memristive mechanism, we systematically investigate the effect of some of the most common defects found in experiments (for instance, sulphur mono- and di-vacancies, adatoms) on the electronic properties of MoS_2 in the vacuum and also in the presence of a metal top contact. Our study constitutes the first step of a wider 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 the detection of gas and small biological molecules, such as glucose.[4] Enzymatic biosensing is the most common approach, however non-enzymatic sensing can provide a higher stability of the sensor and a prompt response, potentially at a lower cost but 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 and electronic properties to assess the possible sensing mechanism. We also study the impact of some of the most used metal dopants employed in lab-scale experiments, such as Ni, Pt, Au, Ag, in order to improve the sensing platform with respect to bare MoS_2.

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

References

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