Exploring supported metal nanoclusters on MoS_2 for the chemical detection of biomolecules in health monitoring wearable devices

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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 technologies. For instance, 2D semiconductors such as single-layer molybdenum disulphide (MoS_2), may provide the ideal platform for the fabrication of field-effect transistors (FETs) with ultra-thin channel, going beyond conventional CMOS technologies [1]. This is due to the material's sizeable band gap of 1.8 eV, its stability, and the possibility given by its reduced dimensionality to control the device channel thickness at the atomic level.

Biosensing is one of the areas in which MoS_2-based transistors can provide significant improvements over devices based on graphene, whose sensitivity was hindered by the material's vanishing band gap. Here we look at MoS_2 as the sensing platform in field-effect biosensors (Bio-FETs) for the detection of complex biomolecules like cortisol. Ultimately, the aim of this study is to design and integrate such biosensors in wearable health monitoring devices [2]. Nevertheless, it is clear that in order to improve the device response towards the analyte of interest, a deep understanding of the material's properties is needed. Therefore, to bridge the gap between materials' properties and device physics we carry out first-principles atomistic computer simulations in the framework of density functional theory (DFT). Our study constitutes the first step of a wider multi-scale modelling approach in which the goal is to construct a full atomistic-to-device level model.

Indeed, MoS_2 has already been studied in the context of biosensors mainly for the detection of gas and small biological molecules, such as glucose and dopamine [3]. Enzymatic biosensing remains 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, the mechanisms that govern the interaction between the analyte and MoS_2 at the molecular level are still far from being understood. Thus, we thoroughly explore the MoS_2/cortisol interaction in terms of structural, electronic, and charge transfer properties to assess possible viable sensing mechanisms. First, we 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 substrate response with respect to pristine MoS_2 [4]. Then, as we strive to increase the complexity of our model, we explore the use of metal nanoclusters (e.g., Pt and Au) to decorate single-layer MoS_2 as yet another mean to detect cortisol, focusing on the clusters size effects.

Overall, our work aims to shed light onto the properties of MoS_2 when used as a biosensor to understand its interaction with cortisol, and to optimize the design of devices towards better performance.

[1] J. A. Robinson, "Perspective: 2D for Beyond CMOS," APL Mater., 6, 058202, **2018**.
[2] EU H2020 SmartVista project, www.smartvista.eu.

[3] G. Jeevanandham et al., “Nickel oxide decorated MoS_2 nanosheet-based non-enzymatic sensor for the selective detection of glucose,” *RSC Adv*., 10, 643-654, **2020**.
[4] G. Boschetto, A. Todri-Sanial, “Assessing doping strategies for monolayer MoS_2 towards non-enzymatic detection of cortisol: a first-principles study,” Phys. Chem. Chem. Phys., **2022**, Advance Article.