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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, together with their ultra-thin size, enable the development of compact devices and innovative 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 conventional CMOS technology. [1]

Here we look at MoS_2 in the context of biosensing, and we study such material as the core component of field-effect biosensors (Bio-FETs) for the detection of cortisol. Ultimately, the aim of this study is to design and integrate such biosensors in wearable health monitoring devices. [2] We want to bridge the gap between materials' properties and device physics and to do so, 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.

Recently, MoS_2 has been studied as a sensing platform for detecting mainly gas and small biological molecules, such as glucose. [3] 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, the mechanisms that govern the interaction between the analyte and MoS_2 at the molecular level are far from being understood. 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 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. In addition to single-atom doping, we also explore the use of metal nanocluster (e.g., Pt and Au) to decorate the MoS_2 layer as yet another mean to detect cortisol.
Overall, our work ultimately aims to obtain a deep understanding of the properties of MoS_2 when used as a sensor to drive the design of devices towards better performance.

References:

1. Y. Qiao et al., *ACS Appl. Electron. Mater.*, **2020**, 2, 346-370.
2. EU H2020 SmartVista project, www.smartvista.eu.
3. G. Jeevanandham et al., *RSC Adv.*, **2020**, 10, 643-654.