Multi-Scale Simulations of Supported Pt Nanoclusters on Single-Layer MoS_2 for Chemiresistive Wearable Biosensors

Gabriele Boschetto,[1] Stefania Carapezzi,[1] Aida Todri-Sanial[1,2]
LIRMM, University of Montpellier, CNRS, Montpellier, France
Department of Electrical Engineering, Eindhoven University of Technology, Eindhoven, Netherlands

The development of non-enzymatic sensors is a challenge which requires, on the one hand, careful design of the sensing materials with respect to the chosen analyte, and on the other hand, suitable device architectures. In this context, atomically-thin two-dimensional (2D) materials have attracted a great deal of interest given their desirable mechanical, electrical and optical properties. For instance, single-layer molybdenum disulfide (MoS2) is an ultra-thin semiconductor which can be used to fabricate devices which go beyond the current state-of-the-art CMOS technology.
Aside from the device level, single-layer MoS2 as a material was also found to be suitable to be used as the sensing platform in FET sensors to detect small molecules (mainly gases) and small biomarkers such as glucose. However, the vast majority of MoS2 FET sensors rely on an enzymatic sensing mechanism, which involves the functionalization of the 2D material with enzymes specific to the chosen analyte. Enzymatic sensors are generally prone to suffer of low stability with respect to temperature and pH.
In this work, we propose single-layer MoS2 decorated with Pt nanoparticles as the non-enzymatic sensing platform for the detection of biomarkers (such as cortisol) in human samples. The aim is to assess the suitability of such a sensing platform for the development of wearable and portable cortisol sensors. We perform multi-scale computer simulations at the materials' level up to device scale. First, ab initio simulations within the framework of density functional theory (DFT) allowed us to gain insights into the interaction, at the atomic level, between the analyte (cortisol) and the sensing platform (MoS2/Pt). Then, by carrying out technology computer-aided design (TCAD) simulations, we were able to consider a device architecture and investigate its performance as cortisol sensor. Following our multi-scale simulation strategy, we were able to propose a FET sensor, whose channel is made of Pt-decorated MoS2. The sensing mechanism relies on the chemiresistive response of the device to the adsorption of cortisol on the channel, which leads to a charge transfer from the analyte to the substrate and, consequently, to the measurable shift in the gate voltage threshold of the FET.
With our findings, we provided important insights and gave our contribution towards the development of highly sensitive non-enzymatic cortisol sensors based on 2D materials.

References

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