Combination of 2D-3D materials with machine learning to detect small ions in complex biological fluids

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Artificial intelligence, and particularly machine learning, are influencing materials science not only in modelling and simulation but also in interpreting complex experimental datasets, such as those generated by **biological sensors** working in matrices like **blood, sweat or saliva**. The "classic" approach in sensor production is to develop highly selective materials which can univocally detect a specific ion or molecule ignoring other interferants; such high selectivity is difficult to obtain, especially in complex matrices.[1]
We propose an alternative strategy based on an array of sensors which, individually, are non-selective, but whose collective response becomes selective thanks to an **artificial neural network (ANN)**. This approach is demonstrated for the **detection of Na^+ and K^+ ions**, two chemically alike species of physiological relevance that lack distinctive electrochemical signatures and are thus hard to differentiate by single sensors. The sensor array combines 2D **graphene oxide (GO)**[2] nanosheets and **3D metal-organic frameworks** (MOF), exploiting the different intercalation and diffusion behaviour of the ions within these materials to generate distinct voltammetric patterns. The ANN is trained on a massive dataset comprising 327 variables and **over four million samples**, enabling accurate determination of ion concentrations from the array response. While an individual sensor is unable to discriminate between Na^+ and K^+, the ANN-guided array achieves reliable quantitative detection.
Neural networks often behave as **black boxes**, providing limited insight into the underlying sensing mechanisms. To get more chemical insight, we further explore the contribution of each sensor by training additional ANNs in which selected electrodes are deliberately excluded. This approach helps elucidate the relative importance of individual sensors in the final analytical output.[3]

References

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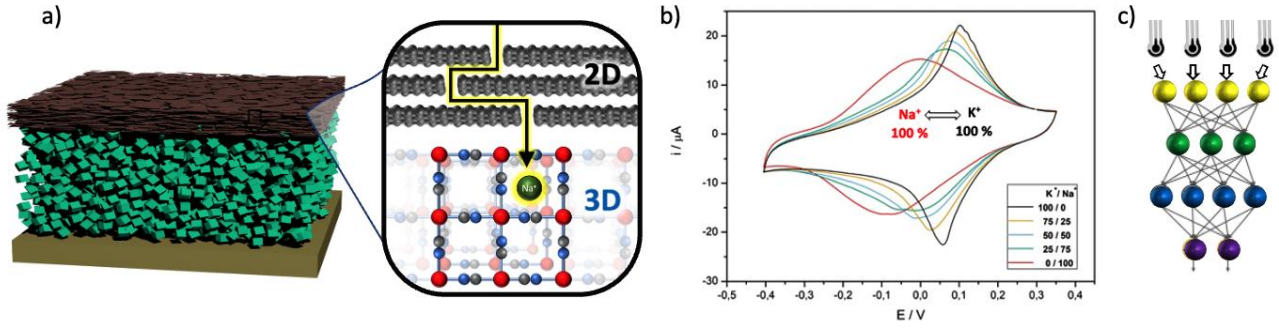

Figure 1: a) Cartoon representing the composite material made of 2-dimensional graphene oxide nanosheets (GO) and 3- dimensional metal-organic frameworks (MOFs). b) Example of cyclic voltammetry curves used to train the neural network (schematized in c).