Multivariate sensing of sodium and potassium ions using Prussian blue, graphene oxide electrodes and machine learning

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The conventional method for sensing relies on the development of highly selective materials capable of detecting specific target molecules or ions without interference from other species commonly found in real solutions. However, creating practical sensors that can effectively discriminate between ions of the same group, which share similar chemistry, presents significant challenges.

To address this issue, we describe a novel approach employing an ensemble of diverse sensor arrays and analysing their multivariate signals to accurately determine the concentrations of Na^+ and K^+ ions in solutions with varying ionic strengths. Our methodology involves utilizing a combination of sensors coated with electrochemically reduced graphene oxide (RGO) and metal-organic frameworks (MOFs), such as iron hexacyanoferrate (also known as Prussian Blue) or nickel hexacyanoferrate. Na^+ and K^+ ions exhibit different intercalation and diffusion behaviours within both RGO and MOFs, resulting in distinct electrochemical signals according to their concentration ratio.

We employ an array of 96 sensors to train an artificial neural network (ANN) capable of analysing such complex inputs. The dataset used for training the ANN consists of 327 variables as columns and over 4 million samples as rows.

Following the training step, the network demonstrates remarkable proficiency in accurately measuring the concentration of either ion present in solution. We could confirm that the combination of the responses deriving from four different electrode coatings results in a prediction accuracy well beyond the use of a single sensor. This ongoing work underscores the potential of integrating artificial intelligence with tunable materials to develop a new class of chemical sensors with enhanced discrimination capabilities, paving the way for more robust and versatile sensor technologies.

References

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Figures

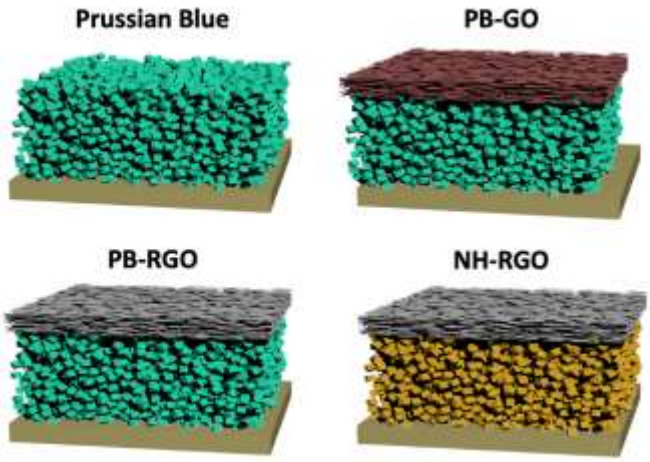

Figure 1. Cartoon showing the different electrode architectures tested in the sensor array.

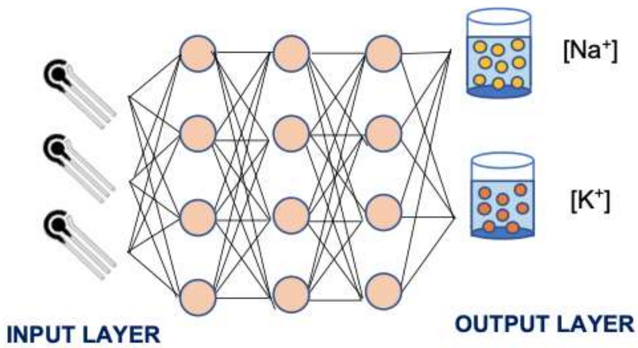

Figure 2. Scheme showing the ANN used to use electrochemical sensor array data to detect concentrations of Na^+ and K^+.